Request Noble Jarrell

Access DB# 150213

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Sabiha Qazi Examiner #: 7414 Date: 4/7/05

Art Unit: 1616 Phone Number 30622 Serial Number: 10/500,532

Mail Box and Bldg/Room Location: 4C70, Rem, 4A45 Results Format Preferred (circle): ~~PAPER~~ DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of invention: Process of Prep. of 1-[3-dimethylamino propyl]-1-(4-fluorophenyl)-1,3-di

Inventors (please provide full names): Rajamannar et al.

Earliest Priority Filing Date: 371 of PCT/IN03/00006. 1/7/03

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search for the process of making isobenzofuran of formula I as in cls 1, 4, 41.

Please attached sheet

Thank you

****

STAFF USE ONLY	Type of Search	Vendors and cost where applicable
Searcher: Noble	NA Sequence (#)	STN 1196
Searcher Phone #:	AA Sequence (#)	Dialog
Searcher Location:	Structure (#) 6 /	Questel/Orbit
Date Searcher Picked Up:	Bibliographic V	Dr.Link
Date Completed 4/11/05	Litigation	Lexis/Nexis
Searcher Prep & Review Time 15	Fulltext	Sequence Systems
Clerical Prep Time:	Patent Family	WWW/Internet
Online Time 73	Other	Other (specify)

PTO-1590 (8-01)

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=> d his

     (FILE 'HOME' ENTERED AT 09:52:34 ON 11 APR 2005)

     FILE 'HCAPLUS' ENTERED AT 09:53:38 ON 11 APR 2005
L1             1 US20050043550/PN
               E IN2002-847/AP,PRN
               E IN2002-MUM847/AP,PRN

     FILE 'WPIX' ENTERED AT 09:59:09 ON 11 APR 2005
L2             1 US20050043550/PN

     FILE 'HCAPLUS' ENTERED AT 10:00:08 ON 11 APR 2005
L3             1 (IN2002-MU847 OR IN2002-MU18 OR IN2002-MU10 OR WO2004-IN6)/AP,P
L4             1 L1 OR L3

     FILE 'REGISTRY' ENTERED AT 10:01:11 ON 11 APR 2005

     FILE 'HCAPLUS' ENTERED AT 10:01:14 ON 11 APR 2005
L5               TRA L4 1- RN :       28 TERMS

     FILE 'REGISTRY' ENTERED AT 10:01:15 ON 11 APR 2005
L6            28 SEA L5

     FILE 'WPIX' ENTERED AT 10:01:19 ON 11 APR 2005
L7             1 (IN2002-MU847 OR IN2002-MU18 OR IN2002-MU10 OR WO2004-IN6)/AP,P
L8             1 L2 OR L7

=> b hcap
FILE 'HCAPLUS' ENTERED AT 10:02:19 ON 11 APR 2005
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FILE COVERS 1907 - 11 Apr 2005  VOL 142 ISS 16
FILE LAST UPDATED: 10 Apr 2005  (20050410/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> d all l4 tot

L4   ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   2003:551309  HCAPLUS
DN   139:117333
ED   Entered STN:  18 Jul 2003
TI   Process for the preparation of 1-[3-(dimethylamino)propyl]-1-(4-
     fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile via cyanation of the
     corresponding chloride or bromide precursors.
IN   Thennati, Rajamannar; Kilaru, Srinivasu; Chinnapillai, Rajendran; Patel,
     Nileshkumar Sureshbhai
PA   Sun Pharmaceutical Industries Limited, India
SO   PCT Int. Appl., 41 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
IC   ICM  A61K
CC   27-7 (Heterocyclic Compounds (One Hetero Atom))
```

FAN. CNT 1

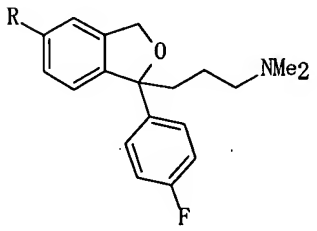
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003057132	A2	20030717	WO 2003-IN6	20030107 <—
	WO 2003057132	A3	20040226		
	WO 2003057132	C1	20040415		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2005043550	A1	20050224	US 2004-500532	20040719 <—
PRAI	IN 2002-MU10	A	20020107 <—		
	IN 2002-MU18	A	20020110 <—		
	IN 2002-MU847	A	20020930 <—		
	WO 2003-IN6	W	20030107		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2003057132	ICM	A61K
US 2005043550	ECLA	C07D307/87B <—

OS CASREACT 139:117333; MARPAT 139:117333

GI



I

AB Title compound (I; R = cyano) (citalopram) was prepared by treatment of I (R = Cl, Br) with a cyanide source in the presence of I- in an amide, amine, or polyether solvent followed by treatment of the crude product containing 1-[3-(methylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile and 5-carboxamido-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)phthalide impurities with a phosphorus oxyhalide, phosphorus oxide cyanide reversal agent, and purification using a solvent system comprising a hydrocarbon and alc., ester, ether, ketone, or mixture thereof. Thus, citalopram containing 4.7% amide and 0.72% desmethylcitalopram impurities was heated with POCl3 in PhMe at 70° for 1 h. The mixture was poured into water and pH was adjusted to 2.0-2.5 with aqueous HCl. The PhMe layer was separated and the pH of the aqueous layer was adjusted to 9.0-9.5 with aqueous NH3 followed by extraction with PhMe to give product containing 0.05% and 0.23% of the amide and desmethylcitalopram resp.

ST citalopram prepn purifn phosphorus oxychloride; halodimethylaminopropylfluorophenyldihydroisobenzofuran cyanation

IT Solvents
(halogenated; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

IT Cyanation catalysts
(iodide ion; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

IT Iodides, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(metal iodides; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

IT Cyanation
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
IT Alcohols, uses
Amides, uses
Amines, uses
Aromatic hydrocarbons, uses
Esters, uses
Ethers, uses
Hydrocarbons, uses
Ketones, uses
Nitriles, uses
Nitro compounds
Polyethers, uses
RL: NUU (Other use, unclassified); USES (Uses)
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
IT 62498-67-3P 64372-56-1P
RL: BYP (Byproduct); PREP (Preparation)
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
IT 59729-32-7P, Citalopram hydrobromide 59729-33-8P, 1-[3-(Dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
IT 60-29-7, Diethyl ether, uses 67-63-0, Isopropanol, uses 67-64-1, Acetone, uses 71-23-8, n-Propanol, uses 108-88-3, Toluene, uses 110-82-7, Cyclohexane, uses 110-86-1, Pyridine, uses 141-78-6, Ethyl acetate, uses 142-82-5, n-Heptane, uses 1330-20-7, Xylene, uses 27175-64-0, Lutidine
RL: NUU (Other use, unclassified); USES (Uses)
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
IT 109-54-6, Dimethylaminopropyl chloride 143-33-9, Sodium cyanide 151-50-8, Potassium cyanide 352-13-6, 4-Fluorophenyl magnesium bromide 460-00-4, 4-Fluorobromobenzene 544-92-3, Cuprous cyanide 19070-16-7 64169-34-2, 5-Bromophthalide 64169-39-7 561304-25-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
IT 1314-56-3, Phosphorus pentoxide, reactions 7681-11-0, Potassium iodide, reactions 10025-87-3, Phosphorus oxychloride
RL: RGT (Reagent); RACT (Reactant or reagent)
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

=> b wpix
FILE 'WPIX' ENTERED AT 10:02:46 ON 11 APR 2005
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FILE LAST UPDATED: 6 APR 2005 <20050406/UP>
MOST RECENT DERWENT UPDATE: 200522 <200522/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

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FOR DETAILS. <<<

=> d all l8 tot

L8 ANSWER 1 OF 1 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2003-636635 [60] WPIX
DNC C2003-174026
TI Preparation of citalopram used as antidepressant agent involves reacting corresponding 5-chloro or bromo derivative with cyanide source.
DC B02
IN CHINNAPILLAI, R; KILARU, S; PATEL, N S; THENNATI, R; RAJAMANNAR, T; RAJENDRAN, C; SRINIVASU, K
PA (SUNP-N) SUN PHARM IND LTD; (PATE-I) PATEL N S; (RAJA-I) RAJAMANNAR T; (RAJE-I) RAJENDRAN C; (SRIN-I) SRINIVASU K
CYC 102
PI WO 2003057132 A2 20030717 (200360)* EN 21 A61K000-00
RW: AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS LU MC MW MZ NL OA PT SD SE SI SK SL SZ TR TZ UG ZM ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT RO RU SC SD SE SG SK SL TJ TM TN TR TT TZ UA UG US UZ VC VN YU ZA ZM ZW
AU 2003222435 A1 20030724 (200421) A61K000-00
US 2005043550 A1 20050224 (200515) C07D307-87 <--
ADT WO 2003057132 A2 WO 2003-IN6 20030107; AU 2003222435 A1 AU 2003-222435 20030107; US 2005043550 A1 WO 2003-IN6 20030107, US 2004-500532 20040719
FDT AU 2003222435 A1 Based on WO 2003057132
PRAI **IN 2002-MU847 20020930; IN 2002-MU10 20020107; IN 2002-MU18 20020110**
IC ICM A61K000-00; C07D307-87
AB WO2003057132 A UPAB: 20031030
NOVELTY - Preparation of citalopram (I) comprises:
(a) reacting the corresponding 5-chloro or bromo derivative (II) with a cyanide source in the presence of iodide and a solvent;
(b) reacting the obtained crude compound with cyanide reversal agent and isolating the base of (I) from the reaction mixture, and
(c) purifying the base from a solvent system.
DETAILED DESCRIPTION - Preparation of citalopram (I) comprises:
(a) reaction of a corresponding 5-chloro or bromo derivative of formula (II) with a cyanide source in the presence of iodide and a solvent (S1);
(b) reacting the obtained crude compound (I) with a cyanide reversal agent, isolating the base of (I) from the reaction mixture and optionally converting (I) into a salt followed by conversion into the base of (I), and
(c) purifying the base from a solvent system comprising a first solvent and second solvent.
R = Br or Cl.
The obtained crude product contains desmethylcitalopram impurity comprising 1-(3-(methylamino)propyl)-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofuran carbonitrile and amide impurity comprising 5-carboxamide-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)-phthalide. The first solvent is hydrocarbon and the second solvent is alcohol, ester, ether and/or ketone. (S1) Comprises amides, amines or polyethers.
INDEPENDENT CLAIMS are also included for:
(1) preparation of (I) by step (a) per se;
(2) preparation of (I) by step (b) per se, where the cyanide reversal agent comprises phosphorus oxyhalides or phosphorus oxides, and
(3) purifying (I) which comprises crystallizing (I) from the solvent system as in step (c).
ACTIVITY - Antidepressant.
No biological data is given.

MECHANISM OF ACTION - None given.
USE - Used as an antidepressant agent (claimed).
ADVANTAGE - High quality (I) is obtained in improved yield by reversing the amide impurity to the desired (I). The process eliminates the use of multiple solvents and operations making it user friendly, and avoids extensive and expensive purification.
Dwg. 0/0
FS CPI
FA AB; GI; DCN
MC CPI: B06-A02; B14-J01A1

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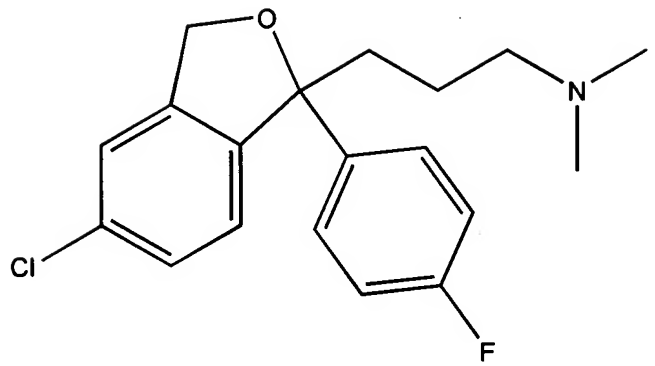

3-(5-chloro-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-1-yl)-*N*,*N*-dimethylpropan-1-amine

$C_{19}H_{21}ClFNO$

=> b reg
FILE 'REGISTRY' ENTERED AT 13:43:13 ON 11 APR 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 APR 2005 HIGHEST RN 848184-66-7
DICTIONARY FILE UPDATES: 10 APR 2005 HIGHEST RN 848184-66-7

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* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
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Crossover limits have been increased. See HELP CROSSOVER for details.

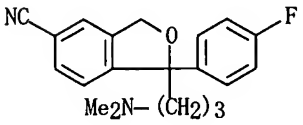
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d ide l9 tot

L9 ANSWER 1 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **500733-84-6** REGISTRY
ED Entered STN: 26 Mar 2003
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, monoacetate (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Citalopram acetate
MF **C20 H21 F N2 O . C2 H4 O2**
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

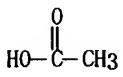
CM 1

CRN 59729-33-8
CMF C20 H21 F N2 O



CM 2

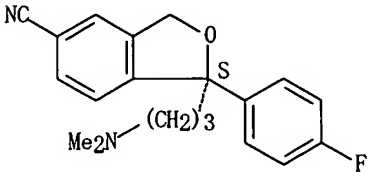
CRN 64-19-7
CMF C2 H4 O2



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 2 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **490037-56-4** REGISTRY
ED Entered STN: 14 Feb 2003
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, labeled with tritium, (1S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C20 H21 F N2 O**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
IL XH-3

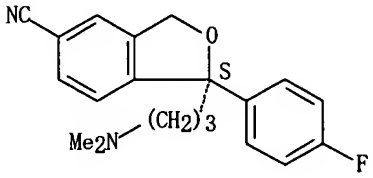
Absolute stereochemistry.



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 3 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **481047-50-1** REGISTRY
ED Entered STN: 24 Jan 2003
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, monohydrobromide, (1S)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (S)-Citalopram hydrobromide
FS STEREOSEARCH
MF **C20 H21 F N2 O . Br H**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
CRN (128196-01-0)

Absolute stereochemistry. Rotation (+).



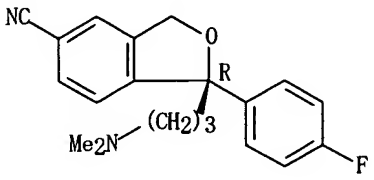
● HBr

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 4 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **481047-49-8** REGISTRY
ED Entered STN: 24 Jan 2003
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, monohydrobromide, (1R)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (R)-Citalopram hydrobromide
FS STEREOSEARCH
MF **C20 H21 F N2 O . Br H**

SR CA
LC STN Files: CA, CAPLUS, USPATFULL
CRN (128196-02-1)

Absolute stereochemistry. Rotation (-).



● HBr

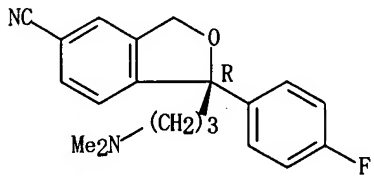
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 5 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **219861-53-7** REGISTRY
ED Entered STN: 21 Feb 1999
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (1R)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)
OTHER NAMES:
CN R-(-)-Citalopram oxalate
FS STEREOSEARCH
MF **C20 H21 F N2 O . C2 H2 O4**
SR CA
LC STN Files: CA, CAPLUS, RTECS*, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

CM 1

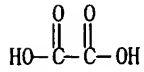
CRN 128196-02-1
CMF C20 H21 F N2 O

Absolute stereochemistry. Rotation (-).



CM 2

CRN 144-62-7
CMF C2 H2 O4



4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

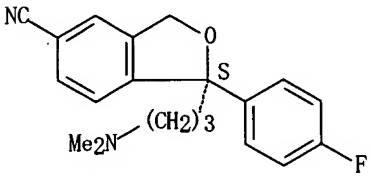
L9 ANSWER 6 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **219861-08-2** REGISTRY
ED Entered STN: 21 Feb 1999

CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (1S)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Cipralex
CN Escitalopram oxalate
CN Lexapro
CN Lu 26-054-0
FS STEREOSEARCH
MF **C20 H21 F N2 O . C2 H2 O4**
CI COM
SR CA
LC STN Files: ADISINSIGHT, BIOSIS, BIOTECHNO, CA, CAPLUS, CHEMCATS, EMBASE, IMSPATENTS, IMSRESEARCH, IPA, MRCK*, PATDPASPC, PROUSDDR, PS, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPATFULL
(*File contains numerically searchable property data)

CM 1

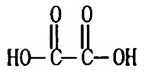
CRN 128196-01-0
CMF C20 H21 F N2 O

Absolute stereochemistry. Rotation (+).



CM 2

CRN 144-62-7
CMF C2 H2 O4

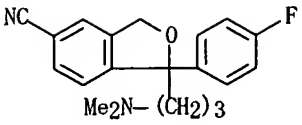


23 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
23 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 7 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **207559-01-1** REGISTRY
ED Entered STN: 24 Jun 1998
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, ethanedioate (1:1) (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (±)-Citalopram oxalate
CN Citalopram oxalate
MF **C20 H21 F N2 O . C2 H2 O4**
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

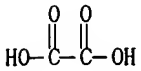
CM 1

CRN 59729-33-8
CMF C20 H21 F N2 O



CM 2

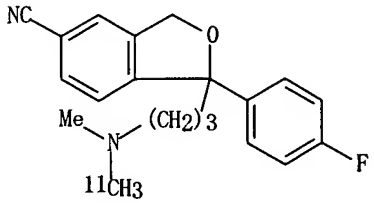
CRN 144-62-7
CMF C2 H2 O4



15 REFERENCES IN FILE CA (1907 TO DATE)
15 REFERENCES IN FILE CAPLUS (1907 TO DATE)

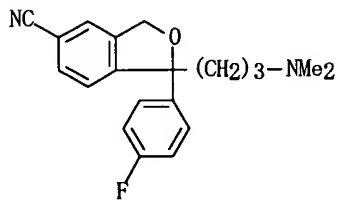
L9 ANSWER 8 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **141258-68-6** REGISTRY
ED Entered STN: 08 May 1992
CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylmethyl-11C-amino)propyl]-, (-)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C20 H21 F N2 O**
SR CA
LC STN Files: CA, CAPLUS

Rotation (-).



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 9 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **135021-05-5** REGISTRY
ED Entered STN: 19 Jul 1991
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, labeled with tritium (9CI) (CA INDEX NAME)
MF **C20 H21 F N2 O**
SR CA
LC STN Files: CA, CAPLUS
IL XH-3



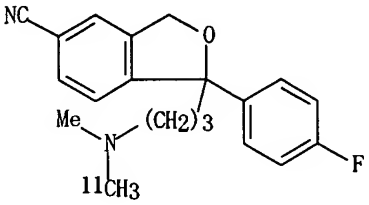
3 REFERENCES IN FILE CA (1907 TO DATE)

Search done by Noble Jarrell

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

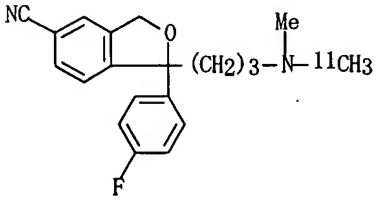
L9 ANSWER 10 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **134915-04-1** REGISTRY
ED Entered STN: 19 Jul 1991
CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylmethyl-11C-amino)propyl]-, (+)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C20 H21 F N2 O**
SR CA
LC STN Files: CA, CAPLUS

Rotation (+).



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

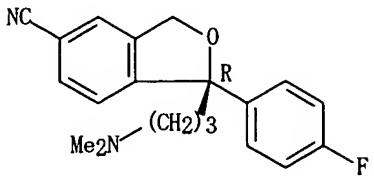
L9 ANSWER 11 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **129356-76-9** REGISTRY
ED Entered STN: 14 Sep 1990
CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylmethyl-11C-amino)propyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C20 H21 F N2 O**
SR CA
LC STN Files: CA, CAPLUS



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 12 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **128196-02-1** REGISTRY
ED Entered STN: 13 Jul 1990
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (1R)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (R)-
OTHER NAMES:
CN (R)-Citalopram
CN R-(-)-Citalopram
FS STEREOSEARCH
MF **C20 H21 F N2 O**
CI COM
SR CA
LC STN Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, IMSPATENTS, IMSRESEARCH, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (-).

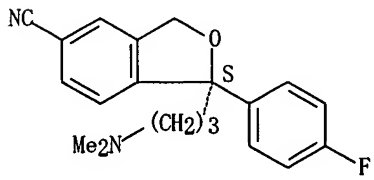


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

46 REFERENCES IN FILE CA (1907 TO DATE)
46 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 13 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **128196-01-0** REGISTRY
ED Entered STN: 13 Jul 1990
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (1S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (S)-
OTHER NAMES:
CN (S)-Citalopram
CN Escitalopram
CN S-(+)-Citalopram
FS STEREOSEARCH
MF **C20 H21 F N2 O**
CI COM
SR CA
LC STN Files: ADISNEWS, ANABSTR, BEILSTEIN*, BIOSIS; BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CHEMCATS, CIN, EMBASE, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MRCK*, PATDPASPC, PHAR, PROMT, PROUSDDR, PS, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

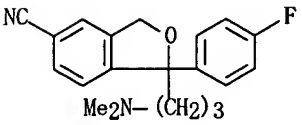
136 REFERENCES IN FILE CA (1907 TO DATE)
136 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 14 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **107190-73-8** REGISTRY
ED Entered STN: 21 Mar 1987
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (E)-2-butenedioate
FS STEREOSEARCH
MF **C20 H21 F N2 O . x C4 H4 O4**
SR CA
LC STN Files: CA, CAPLUS, IMSPATENTS, IMSRESEARCH, PS

Search done by Noble Jarrell

CM 1

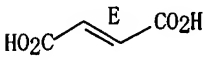
CRN 59729-33-8
CMF C20 H21 F N2 O



CM 2

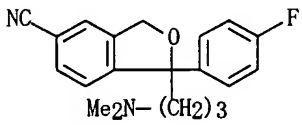
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 15 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **85118-27-0** REGISTRY
ED Entered STN: 16 Nov 1984
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (±)-Citalopram hydrochloride
CN Citalopram hydrochloride
DR 316121-47-8
MF **C20 H21 F N2 O . Cl H**
CI COM
SR European Union (EU)
LC STN Files: CA, CAPLUS, CHEMLIST, PS, TOXCENTER, USPAT2, USPATFULL
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
CRN (59729-33-8)



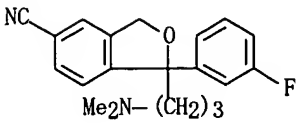
● HCl

13 REFERENCES IN FILE CA (1907 TO DATE)
13 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 16 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **64372-51-6** REGISTRY
ED Entered STN: 16 Nov 1984
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(3-fluorophenyl)-1,3-dihydro-, ethanedioate (1:1) (9CI) (CA INDEX NAME)
MF **C20 H21 F N2 O . C2 H2 O4**
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

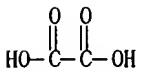
CM 1

CRN 64372-50-5
CMF C20 H21 F N2 O



CM 2

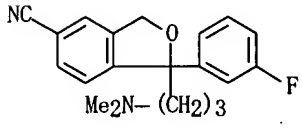
CRN 144-62-7
CMF C2 H2 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 17 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **64372-50-5** REGISTRY
ED Entered STN: 16 Nov 1984
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(3-fluorophenyl)-1,3-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C20 H21 F N2 O**
CI COM
LC STN Files: BEILSTEIN*
(*File contains numerically searchable property data)

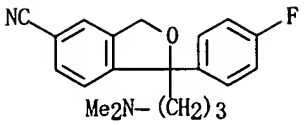


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 ANSWER 18 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **64169-59-1** REGISTRY
ED Entered STN: 16 Nov 1984
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, ethanedioate (9CI) (CA INDEX NAME)
MF **C20 H21 F N2 O . x C2 H2 O4**
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, IMSPATENTS, IMSRESEARCH, USPATFULL

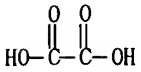
CM 1

CRN 59729-33-8
CMF C20 H21 F N2 O



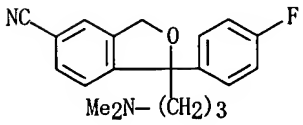
CM 2

CRN 144-62-7
CMF C2 H2 O4



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 19 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **59729-33-8** REGISTRY
ED Entered STN: 16 Nov 1984
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (±)-Citalopram
CN 1-[3-(Dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-5-carbonitrile
CN Bonitrile
CN Citalopram
CN Lu 10-171
CN Nitalapram
FS 3D CONCORD
DR 128196-03-2, 103146-27-6
MF **C20 H21 F N2 O**
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DIOGENES, DRUGU, EMBASE, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE, MRCK*, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)

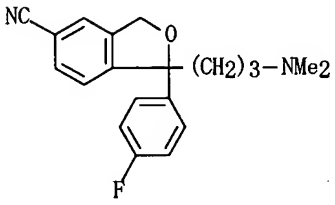


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1438 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1443 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 20 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN
RN **59729-32-7** REGISTRY
ED Entered STN: 16 Nov 1984

CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, monohydrobromide (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (±)-Citalopram hydrobromide
CN Apertia
CN Celexa
CN Cipram
CN Cipramil
CN Citalopram hydrobromide
CN Elopram
CN Lu 10-171B
CN Lupram
CN Prisdal
CN Sepram
CN Seropram
MF **C20 H21 F N2 O . Br H**
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMLIST, CIN, DIOGENES, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSPATENTS, IMSRESEARCH, IPA, MRCK*, PHAR, PIRA, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
CRN (59729-33-8)



● HBr

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

81 REFERENCES IN FILE CA (1907 TO DATE)
81 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide l10 tot

L10 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 488148-14-7 REGISTRY
ED Entered STN: 10 Feb 2003
CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, (1S)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (S)-(+)-1-(4-Fluorophenyl)-1-[3-(dimethylamino)propyl]-5-bromophthalane
FS STEREOSEARCH
MF **C19 H21 Br F N O**
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry. Rotation (+).

IT **59729-32-7P, Citalopram** hydrobromide **59729-33-8P**
, 1-[3-(Dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile
RL: **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(process for the preparation of **citalopram** via cyanation of the corresponding chloride or bromide precursor)

IT 60-29-7, Diethyl ether, uses 67-63-0, Isopropanol, uses 67-64-1, Acetone, uses 71-23-8, n-Propanol, uses 108-88-3, Toluene, uses 110-82-7, Cyclohexane, uses 110-86-1, Pyridine, uses 141-78-6, Ethyl acetate, uses 142-82-5, n-Heptane, uses 1330-20-7, Xylene, uses 27175-64-0, Lutidine
RL: NUU (Other use, unclassified); USES (Uses)
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

IT 109-54-6, Dimethylaminopropyl chloride 143-33-9, Sodium cyanide 151-50-8, Potassium cyanide 352-13-6, 4-Fluorophenyl magnesium bromide 460-00-4, 4-Fluorobromobenzene 544-92-3, Cuprous cyanide 19070-16-7 64169-34-2, 5-Bromophthalide **64169-39-7 561304-25-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

IT 1314-56-3, Phosphorus pentoxide, reactions 7681-11-0, Potassium iodide, reactions 10025-87-3, Phosphorus oxychloride
RL: RGT (Reagent); RACT (Reactant or reagent)
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

=> d all hitrn 169 tot

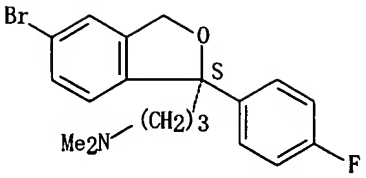
L69 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:691476 HCAPLUS
DN 141:207048
ED Entered STN: 25 Aug 2004
TI Preparation of pure citalopram
IN Kaushik, Vipin Kumar; Rao, Divvela Venkata Naga Srinivasa; Handa, Vijay Kumar; Sivakumaran, Meenakshisunderam
PA Aurobindo Pharma Ltd., India
SO U.S., 3 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07D307-78
NCL 549467000; 549469000
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6781003	B1	20040824	US 2003-456135	20030609
PRAI	US 2003-456135		20030609		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6781003	ICM	C07D307-78
	NCL	549467000; 549469000
US 6781003	ECLA	C07D307/81

OS CASREACT 141:207048
GI

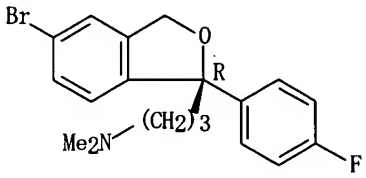


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 488148-13-6 REGISTRY
ED Entered STN: 10 Feb 2003
CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, (1R)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (R)-(-)-1-(4-Fluorophenyl)-1-[3-(dimethylamino)propyl]-5-bromophthalane
FS STEREOSEARCH
MF **C19 H21 Br F N O**
SR CA
LC STN Files: CA, CAPLUS

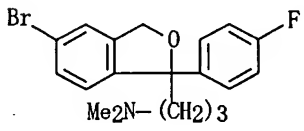
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 479065-02-6 REGISTRY
ED Entered STN: 15 Jan 2003
CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, hydrobromide (9CI) (CA INDEX NAME)
MF **C19 H21 Br F N O . Br H**
SR CA
LC STN Files: CA, CAPLUS, CASREACT
CRN (64169-39-7)



● HBr

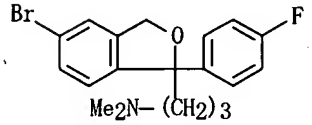
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Search done by Noble Jarrell

L10 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 64372-43-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)
MF **C19 H21 Br F N O . C2 H2 O4**
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

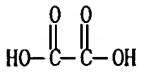
CM 1

CRN 64169-39-7
CMF C19 H21 Br F N O



CM 2

CRN 144-62-7
CMF C2 H2 O4



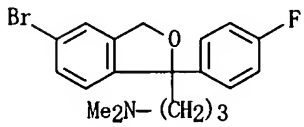
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 64169-40-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)
MF **C19 H21 Br F N O . x C2 H2 O4**
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

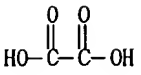
CM 1

CRN 64169-39-7
CMF C19 H21 Br F N O



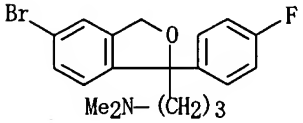
CM 2

CRN 144-62-7
CMF C2 H2 O4



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 64169-39-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-(4-Fluorophenyl)-1-(3-dimethylaminopropyl)-5-bromophthalane
CN 5-Bromo-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran
FS 3D CONCORD
DR 561304-26-5
MF **C19 H21 Br F N O**
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, USPAT2, USPATFULL
(*File contains numerically searchable property data)

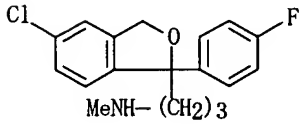


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

20 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
20 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide l11 tot

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN 561304-25-4 REGISTRY
ED Entered STN: 06 Aug 2003
CN 1-Isobenzofuranpropanamine, 5-chloro-1-(4-fluorophenyl)-1,3-dihydro-N-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF **C18 H19 Cl F N O**
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

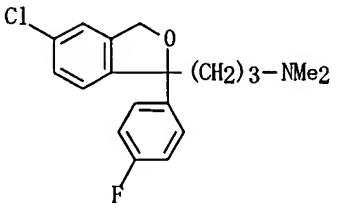


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide l13 tot

L13 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN
RN **64169-47-7** REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Isobenzofuranpropanamine, 5-chloro-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)
MF **C19 H21 Cl F N O . Cl H**
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
CRN (64169-45-5)



● HCl

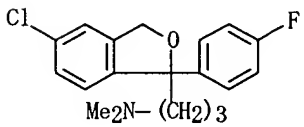
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L13 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN
RN **64169-46-6** REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Isobenzofuranpropanamine, 5-chloro-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)
MF **C19 H21 Cl F N O . x C2 H2 O4**
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

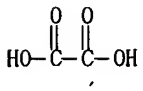
CM 1

CRN 64169-45-5
CMF C19 H21 Cl F N O



CM 2

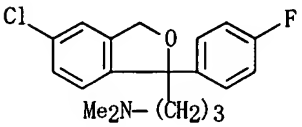
CRN 144-62-7
CMF C2 H2 O4



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L13 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN
RN **64169-45-5** REGISTRY
ED Entered STN: 16 Nov 1984

CN 1-Isobenzofuranpropanamine, 5-chloro-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-(4-Fluorophenyl)-1-(3-dimethylaminopropyl)-5-chlorophthalane
CN Lu 10-134C
FS 3D CONCORD
DR 843660-63-9
MF **C19 H21 Cl F N O**
CI COM
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

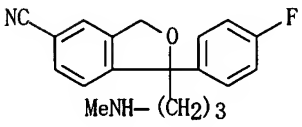
12 REFERENCES IN FILE CA (1907 TO DATE)
12 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide l17 tot

L17 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 526204-73-9 REGISTRY
ED Entered STN: 06 Jun 2003
CN **5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (9CI)** (CA INDEX NAME)
FS STEREOSEARCH
MF **C19 H19 F N2 O . C4 H6 O6**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

CM 1

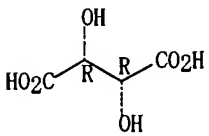
CRN 62498-67-3
CMF C19 H19 F N2 O



CM 2

CRN 87-69-4
CMF C4 H6 O6

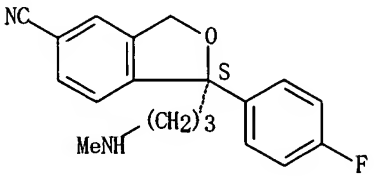
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 144025-14-9 REGISTRY
ED Entered STN: 21 Oct 1992
CN **5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, (1S)- (9CI)** (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN **5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, (S)-**
OTHER NAMES:
CN (S)-(+)-N-Demethylcitalopram
CN **(S)-1-(3-Methylaminopropyl)-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-5-carbonitrile**
CN (S)-Desmethylcitalopram
FS STEREOSEARCH
MF **C19 H19 F N2 O**
SR CA
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (+).

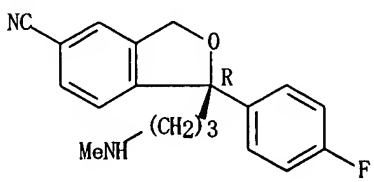


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

25 REFERENCES IN FILE CA (1907 TO DATE)
25 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 144010-85-5 REGISTRY
ED Entered STN: 16 Oct 1992
CN **5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, (1R)- (9CI)** (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN **5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, (R)-**
OTHER NAMES:
CN (R)-(-)-N-Demethylcitalopram
CN (R)-Desmethylcitalopram
FS STEREOSEARCH
MF **C19 H19 F N2 O**
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

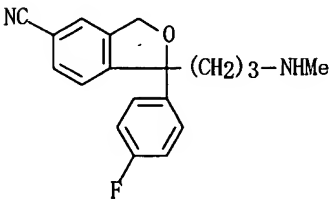
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

19 REFERENCES IN FILE CA (1907 TO DATE)
19 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 97743-99-2 REGISTRY
ED Entered STN: 24 Aug 1985
CN **5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, monohydrochloride (9CI)** (CA INDEX NAME)
OTHER NAMES:
CN Lu 11-109C
MF **C19 H19 F N2 O . Cl H**
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
CRN (62498-67-3)



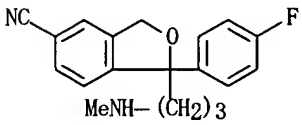
● HCl

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 62498-68-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN **5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, ethanedioate (1:1) (9CI)** (CA INDEX NAME)
MF **C19 H19 F N2 O . C2 H2 O4**
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPAT2, USPATFULL
(*File contains numerically searchable property data)

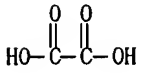
CM 1

CRN 62498-67-3
CMF C19 H19 F N2 O



CM 2

CRN 144-62-7
CMF C2 H2 O4

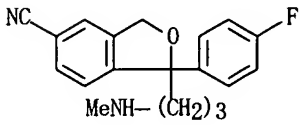


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Search done by Noble Jarrell

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 62498-67-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN **5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]- (9CI)** (CA INDEX NAME)
OTHER NAMES:
CN (±)-N-Demethylcitalopram
CN Demethylcitalopram
CN Desmethylcitalopram
CN Lu 11-109
CN Norcitalopram
CN Rac-Desmethylcitalopram
FS 3D CONCORD
DR 144070-76-8
MF **C19 H19 F N2 O**
CI COM
LC STN Files: ADISNEWS, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CHEMLIST, DDFU, DRUGU, EMBASE, IPA, MEDLINE, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)

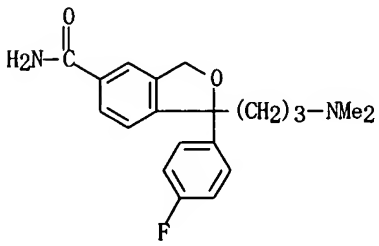


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

108 REFERENCES IN FILE CA (1907 TO DATE)
110 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide l19 tot

L19 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN 64372-56-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN **5-Isobenzofurancarboxamide, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro- (9CI)** (CA INDEX NAME)
FS 3D CONCORD
MF **C20 H23 F N2 O2**
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPAT2, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide 145 tot

L45 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN 7681-11-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Potassium iodide (KI) (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Antistrumin
CN Asmofug E
CN Ceoiodin
CN Iodostin
CN Jodid
CN K1-N
CN Kaiod
CN Knollide
CN NSC 77362
CN Pherajod
CN **Potassium iodide**
CN Potassium monoiodide
CN Thyro-Block
CN Thyrojod
DR 59216-96-5, 106449-25-6, 61456-02-8, 39448-53-8
MF I K
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIOGENES, DIPPR*, DRUGU, EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, TOXCENTER, TULSA, ULIDAT, USAN, USPAT2, USPATFULL, VETU, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

I-K

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

19901 REFERENCES IN FILE CA (1907 TO DATE)
199 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
19915 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide 148 tot

L48 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 438043-97-1 REGISTRY
ED Entered STN: 10 Jul 2002
CN **Copper cyanide (63Cu(C15N)) (9CI)** (CA INDEX NAME)
MF **C Cu N**
SR CA
LC STN Files: CA, CAPLUS

$^{63}Cu-C\equiv{}^{15}N$

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 438043-96-0 REGISTRY
ED Entered STN: 10 Jul 2002

CN **Copper cyanide (63Cu(13CN)) (9CI)** (CA INDEX NAME)
MF **C Cu N**
SR CA
LC STN Files: CA, CAPLUS

$^{63}Cu-^{13}C\equiv N$

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 438043-95-9 REGISTRY
ED Entered STN: 10 Jul 2002
CN **Copper cyanide (65Cu(CN)) (9CI)** (CA INDEX NAME)
MF **C Cu N**
SR CA
LC STN Files: CA, CAPLUS

$^{65}Cu-C\equiv N$

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 438043-94-8 REGISTRY
ED Entered STN: 10 Jul 2002
CN **Copper cyanide (63Cu(CN)) (9CI)** (CA INDEX NAME)
MF **C Cu N**
SR CA
LC STN Files: CA, CAPLUS

$^{63}Cu-C\equiv N$

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 204571-13-1 REGISTRY
ED Entered STN: 24 Apr 1998
CN **Copper cyanide (Cu(C15N)) (9CI)** (CA INDEX NAME)
OTHER NAMES:
CN Cuprous cyanide-15N
MF **C Cu N**
SR CA
LC STN Files: CA, CAPLUS, CHEMCATS

$Cu-C\equiv{}^{15}N$

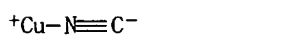
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 199450-10-7 REGISTRY
ED Entered STN: 07 Jan 1998
CN **Copper cyanide (Cu(13C15N)) (9CI)** (CA INDEX NAME)
MF **C Cu N**
SR CA
LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM

$Cu-^{13}C\equiv{}^{15}N$

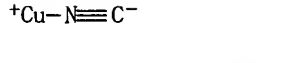
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 188592-60-1 REGISTRY
ED Entered STN: 24 Apr 1997
CN **Copper cyanide (Cu(NC)), monohydrogen (9CI)** (CA INDEX NAME)
MF **C Cu N . H**
CI CCS
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
CRN (147023-48-1)



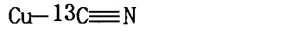
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 147023-48-1 REGISTRY
ED Entered STN: 16 Apr 1993
CN **Copper cyanide (Cu(NC)) (9CI)** (CA INDEX NAME)
MF **C Cu N**
CI CCS, COM
SR CA
LC STN Files: CA, CAPLUS, CASREACT



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 93596-81-7 REGISTRY
ED Entered STN: 18 Dec 1984
CN **Copper cyanide (Cu(13CN)) (9CI)** (CA INDEX NAME)
OTHER NAMES:
CN Cuprous cyanide-13C
MF **C Cu N**
LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM



11 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 17410-52-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN **Copper cyanide (Cu(14CN)) (8CI, 9CI)** (CA INDEX NAME)
OTHER NAMES:
CN Copper(I) [14C]cyanide
CN Cuprous cyanide-14C
CN Cuprous cyanide-14C (Cu14CN)
CN Hydrocyanic-14C acid, copper(1+) salt
DR 98259-65-5, 35947-46-7, 68378-43-8, 78825-27-1
MF **C Cu N**
LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, TOXCENTER, USPATFULL

Cu–^{14}C≡N

29 REFERENCES IN FILE CA (1907 TO DATE)
29 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 6023-28-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN **Copper cyanide (Cu(CN)), monoammoniate (8CI)** (CA INDEX NAME)
MF **C Cu N . H3 N**
LC STN Files: GMELIN*
(*File contains numerically searchable property data)
CRN (544-92-3)

Cu–C≡N

● NH_3

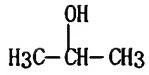
L48 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 544-92-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN **Copper cyanide (Cu(CN)) (6CI, 7CI, 8CI, 9CI)** (CA INDEX NAME)
OTHER NAMES:
CN **Copper cyanide**
CN **Copper monocyanide**
CN **Copper(1+) cyanide**
CN **Copper(I) cyanide**
CN Cupricin
CN Cuprous cyanide
DR 13092-67-6
MF **C Cu N**
CI COM
LC STN Files: ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DETHERM*, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PROMT, PS, RTECS*, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

Cu–C≡N

1445 REFERENCES IN FILE CA (1907 TO DATE)
16 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1447 REFERENCES IN FILE CAPLUS (1907 TO DATE)
39 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> => d ide l63 tot

L63 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN
RN 70504-57-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Propanol, aluminum nickel(2+) salt (8:2:1) (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Nickel bis(tetraisopropanolatoaluminate(1-))**
MF **C3 H8 O . 1/4 Al . 1/8 Ni**
LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL
CRN (67-63-0)

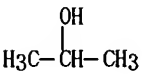


●1/4 Al

●1/8 Ni(II)

8 REFERENCES IN FILE CA (1907 TO DATE)
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

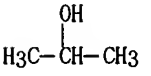
L63 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN
RN 30429-72-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Propanol, holmium(3+) salt (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **Isopropanol, holmium(3+) salt**
MF **C3 H8 O . 1/3 Ho**
LC STN Files: CA, CAPLUS, CHEMCATS, USPATFULL
CRN (67-63-0)



●1/3 Ho(III)

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L63 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN
RN 6831-82-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Propanol, potassium salt (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Isopropyl alcohol, potassium salt (8CI)
CN Potassium isopropoxide (6CI, 7CI)
OTHER NAMES:
CN **Potassium isopropanolate**
CN Potassium isopropylate
MF **C3 H8 O . K**
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, GMELIN*, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
CRN (67-63-0)

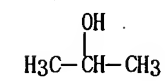


● K

Search done by Noble Jarrell

170 REFERENCES IN FILE CA (1907 TO DATE)
171 REFERENCES IN FILE CAPLUS (1907 TO DATE)
14 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

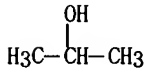
L63 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN
RN 6742-69-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Propanol, ytterbium(3+) salt (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Isopropyl alcohol, ytterbium(3+) salt (8CI)
CN Ytterbium isopropoxide (Yb(OC3H7)3) (7CI)
OTHER NAMES:
CN **Tris(isopropanolato)ytterbium**
CN Tris(isopropoxo)ytterbium
CN Ytterbium triisopropoxide
MF **C3 H8 O . 1/3 Yb**
CI COM
LC STN Files: CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM, GMELIN*, IFICDB, IFIPAT, IFIUDB, USPAT2, USPATFULL
(*File contains numerically searchable property data)
CRN (67-63-0)



●1/3 Yb(III)

79 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
80 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

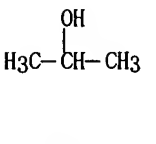
L63 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN
RN 2388-10-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Propanol, lithium salt (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Isopropyl alcohol, lithium salt (8CI)
CN Lithium isopropoxide (6CI, 7CI)
OTHER NAMES:
CN **Isopropanol lithium salt**
CN Isopropoxylithium
CN **Lithium isopropanolate**
CN Lithium isopropylate
MF **C3 H8 O . Li**
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
CRN (67-63-0)



● Li

168 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
168 REFERENCES IN FILE CAPLUS (1907 TO DATE)
10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

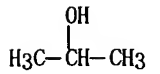
L63 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN
RN 683-60-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Propanol, sodium salt (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Isopropyl alcohol, sodium salt (8CI)
CN Sodium isopropoxide (6CI, 7CI)
OTHER NAMES:
CN **Isopropanol sodium salt**
CN Isopropoxysodium
CN **Sodium isopropanolate**
CN Sodium isopropyl oxide
CN Sodium isopropylate
MF **C3 H8 O . Na**
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, GMELIN*, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
CRN (67-63-0)



543 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
545 REFERENCES IN FILE CAPLUS (1907 TO DATE)
32 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L63 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN
RN 555-31-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Propanol, aluminum salt (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Isopropyl alcohol, aluminum salt (8CI)
OTHER NAMES:
CN AIPD
CN Aliso
CN Aluminium isopropoxide
CN Aluminum 2-propoxide
CN **Aluminum isopropanolate**
CN Aluminum isopropioate
CN Aluminum isopropoxide
CN Aluminum isopropoxide (1:3)
CN Aluminum isopropylate
CN Aluminum isopropylate (Al(OC3H7)3)
CN Aluminum sec-propanolate
CN Aluminum triisopropoxide
CN Aluminum triisopropylate
CN Aluminum tris(iso-propoxide)
CN Aluminum tris(isopropoxide)
CN Aluminum tris(isopropylate)
CN Aluminum tris(sec-propoxide)
CN Aluminum(3+) isopropoxide
CN **Isopropanol aluminum salt**
CN Manalox 130
CN PADM
CN Triisopropoxyaluminum

CN Triisopropyl aluminate
CN Triisopropyloxyaluminum
CN Tris(isopropoxy)aluminum
DR 12343-27-0, 95797-38-9, 51796-09-9, 78423-41-3, 188398-62-1, 245654-30-2, 301192-92-7, 358732-16-8, 365494-41-3
MF **C3 H8 O . 1/3 Al**
CI COM
LC STN Files: AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DETHERM*, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MRCK*, MSDS-OHS, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
CRN (67-63-0)

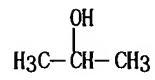


●1/3 Al

3870 REFERENCES IN FILE CA (1907 TO DATE)
207 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3873 REFERENCES IN FILE CAPLUS (1907 TO DATE)
78 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L63 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN
RN 546-68-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Isopropyl alcohol, titanium(4+) salt (8CI)
CN Titanium isopropoxide (Ti(OC3H7)4) (7CI)
OTHER NAMES:
CN 5N
CN 5N (titanate)
CN A 1
CN A 1 (titanate)
CN Isopropyl orthotitanate
CN Isopropyl titanate(IV) ((C3H7O)4Ti)
CN Orgatix TA 10
CN TA 10
CN **Tetraisopropanolatotitanium**
CN Tetraisopropoxytitanium
CN Tetraisopropoxytitanium(IV)
CN Tetraisopropyl orthotitanate
CN Tetraisopropyl titanate
CN **Tetrakis(isopropanolato)titanium**
CN Tetrakis(isopropoxy)titanium
CN Tetrakis(isopropylato)titanium(IV)
CN Tetrakis(isopropyloxy)titanium
CN Tilcom TIPT
CN Titanium isopropoxide
CN Titanium isopropylate
CN Titanium tetraisopropoxide
CN Titanium tetraisopropylate
CN Titanium tetrakis(iso-propoxide)
CN Titanium tetrakis(isopropoxide)
CN Titanium(4+) isopropoxide
CN Titanium(IV) isopropoxide
CN Titanium, tetrakis(1-methylethoxy)-
CN TPT
CN Tyzor TPT
CN Vertec TIPT

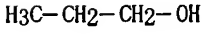
DR 505093-57-2, 176680-01-6, 167709-32-2, 128796-34-9, 131530-94-4, 94340-28-0, 3651-85-2, 119651-13-7, 112797-74-7, 73264-97-8, 71515-81-6, 147809-57-2, 50336-56-6, 118815-04-6, 186518-71-8, 187601-75-8, 195382-13-9, 198699-88-6, 210407-18-4, 216859-04-0, 244173-55-5, 245654-31-3, 255839-65-7, 259264-35-2, 310882-94-1, 347859-73-8, 366477-01-2, 408306-55-8, 518050-49-2
MF **C3 H8 O . 1/4 Ti**
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DETHERM*, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, PIRA, PROMT, RTECS*, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
CRN (67-63-0)



●1/4 Ti(IV)

8443 REFERENCES IN FILE CA (1907 TO DATE)
454 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
8458 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

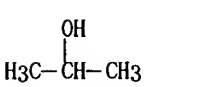
L63 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN
RN 71-23-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Propanol (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Propyl alcohol (8CI)
OTHER NAMES:
CN 1-Hydroxypropane
CN Ethylcarbinol
CN **n-Propanol**
CN n-Propyl alcohol
CN NSC 30300
CN Optal
CN Osmosol extra
CN Propanol
FS 3D CONCORD
MF **C3 H8 O**
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VETU, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

30692 REFERENCES IN FILE CA (1907 TO DATE)
465 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
30718 REFERENCES IN FILE CAPLUS (1907 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L63 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN
RN 67-63-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Propanol (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Isopropyl alcohol (8CI)
OTHER NAMES:
CN 1-Methylethanol
CN 1-Methylethyl alcohol
CN 2-Hydroxypropane
CN 2-Propyl alcohol
CN Alcojel
CN Alcosolve 2
CN Autosept
CN Avantin
CN Avantine
CN Combi-Schutz
CN Dimethylcarbinol
CN Hartosol
CN Imsol A
CN IPA
CN IPS 1
CN IPS 1 (alcohol)
CN iso-Propanol
CN iso-Propyl alcohol
CN Isohol
CN **Isopropanol**
CN Lutosol
CN n-Propan-2-ol
CN NSC 135801
CN Petrohol
CN PRO
CN Propol
CN sec-Propanol
CN sec-Propyl alcohol
CN Sterisol Hand Disinfectant
CN Takineocol
CN Tokuso IPA
CN Virahol
FS 3D CONCORD
DR 8013-70-5
MF **C3 H8 O**
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIOGENES, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USAN, USPAT2, USPATFULL, VETU, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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          48960 REFERENCES IN FILE CA (1907 TO DATE)
            816 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
          49038 REFERENCES IN FILE CAPLUS (1907 TO DATE)
              8 REFERENCES IN FILE CAOLD (PRIOR TO 1967)


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     (FILE 'HOME' ENTERED AT 13:27:33 ON 11 APR 2005)

     FILE 'HCAPLUS' ENTERED AT 13:27:40 ON 11 APR 2005
L1             1 SEA ABB=ON  PLU=ON  US20050043550/PN
L2             1 SEA ABB=ON  PLU=ON  (IN2002-MU847 OR IN2002-MU18 OR IN2002-MU10
                 OR WO2003-IN6)/AP,PRN
L3             1 SEA ABB=ON  PLU=ON  (L1 OR L2)

     FILE 'REGISTRY' ENTERED AT 13:29:08 ON 11 APR 2005

     FILE 'HCAPLUS' ENTERED AT 13:29:10 ON 11 APR 2005
L4               TRA L3 1- RN :       28 TERMS

     FILE 'REGISTRY' ENTERED AT 13:29:10 ON 11 APR 2005
L5            28 SEA ABB=ON  PLU=ON  L4
L6               QUE ABB=ON  PLU=ON  (PMS OR MAN OR IDS)/CI OR UNSPECIFIED OR
                 COMPOUND OR COMPD OR (D OR T)/ELS
L7            27 SEA ABB=ON  PLU=ON  C20H21FN2O AND OC4-C6/ES AND 46.150.18/RID
                 AND NR=3
L8            22 SEA ABB=ON  PLU=ON  L7 NOT L6
                 SEL RN 1-4 7-22 L8
L9            20 SEA ABB=ON  PLU=ON  (107190-73-8/BI OR 128196-01-0/BI OR
                 128196-02-1/BI OR 129356-76-9/BI OR 134915-04-1/BI OR 135021-05
                 -5/BI OR 141258-68-6/BI OR 207559-01-1/BI OR 219861-08-2/BI OR
                 219861-53-7/BI OR 481047-49-8/BI OR 481047-50-1/BI OR 490037-56
                 -4/BI OR 500733-84-6/BI OR 59729-32-7/BI OR 59729-33-8/BI OR
                 64169-59-1/BI OR 64372-50-5/BI OR 64372-51-6/BI OR 85118-27-0/B
                 I) AND L8
                 D SCA
L10            6 SEA ABB=ON  PLU=ON  C19H21BRFNO AND OC4-C6/ES AND 46.150.18/RID
                  AND NR=3
                 D SCA
L11            1 SEA ABB=ON  PLU=ON  C18H19CLFNO AND OC4-C6/ES AND 46.150.18/RID
                  AND NR=3
                 D SCA
L12            6 SEA ABB=ON  PLU=ON  C19H21CLFNO AND OC4-C6/ES AND 46.150.18/RID
                  AND NR=3
                 D STR TOT
                 SEL RN 4-6 L12
L13            3 SEA ABB=ON  PLU=ON  (64169-45-5/BI OR 64169-46-6/BI OR
                 64169-47-7/BI) AND L12
L14            8 SEA ABB=ON  PLU=ON  C19H19FN2O AND OC4-C6/ES AND 46.150.18/RID
                 AND NR=3
                 D SCA
L15            7 SEA ABB=ON  PLU=ON  L14 NOT (D OR T)/ELS
L16            7 SEA ABB=ON  PLU=ON  L15 AND METHYLAMINO
L17            6 SEA ABB=ON  PLU=ON  L16 NOT DIMETHYLAMINO
L18            7 SEA ABB=ON  PLU=ON  C20H23FN2O2 AND OC4-C6/ES AND 46.150.18/RID
                  AND NR=3
                 D SCA
L19            1 SEA ABB=ON  PLU=ON  ISOBENZOFURANCARBOXAMIDE AND L18

     FILE 'HCAPLUS' ENTERED AT 13:53:58 ON 11 APR 2005
L20           93 SEA ABB=ON  PLU=ON  (L9 OR ?CITALOPRAM/BI OR CIPRALEX OR
                 LEXAPRO OR LU (1A) (260540 OR 26 (1A) 0540 OR 26 (1A) 054?) OR
                 LU26054? OR LU26 (1A) 540 OR BONITRILE OR LU10171 OR LU10 (1A)
                 171 OR LU (1A) (10171 OR 10 (1A) 171) OR NITRALAPRAM OR
                 APERTIA OR CELEXA OR CIPRAM) (L) PREP+NT/RL
L21            0 SEA ABB=ON  PLU=ON  (CIPRAMIL# OR ELOPRAM# OR LUPRAM OR
                 PRISDAL# OR SEPRAM# OR SEROPRAM# OR LU10171B OR LU10 (1A) 171B
                 OR LU(1A) (10171B OR 10 (1A) 171B OR 10171 (1A) B OR 10 (1A)
```

```
            171 (1A) B))(L) PREP+NT/RL
L22          32 SEA ABB=ON  PLU=ON  L10 OR L11 OR L13 OR FLUOROPHENYL (2A)(DIME
                THYLAMINO OR DIMETHYL (1A) AMINO OR DI (1A) METHYL (1A) AMINO
                OR DI (1A) METHYLAMINO) (1A) PROPYL (1A)BROMOPHTHALENE
L23         412 SEA ABB=ON  PLU=ON  BROMO (1A)(DIMETHYLAMINO OR DIMETHYL (1A)
                AMINO OR DI (1A) (METHYLAMINO OR METHYL (1A) AMINO) (2A)
                FLUOROPHENYL (2A)(DIHYDROISOBENZOFURAN OR DI (1A) (HYDROISOBENZ
                OFURAN OR HYDRO (1A) (ISOBENZOFURAN OR ISO (1A) (BENZOFURAN OR
                BENZO(1A)FURAN)))))
L24           3 SEA ABB=ON  PLU=ON  LU10134C OR LU (1A) (10134C OR 10 (1A)
                134C OR 10 (1A) 134 (1A) C)
L25          26 SEA ABB=ON  PLU=ON  L20 AND (L22 OR L23 OR L24)
L26             QUE ABB=ON  PLU=ON  PY<=2003 OR AY<=2003 OR PRY<=2003
                E RAJAMANNAR T/AU
L27          20 SEA ABB=ON  PLU=ON  ("RAJAMANNAR T"/AU OR "RAJAMANNAR THENNATI"
                /AU)
                E SRINVASU K/AU
                E SRINIVASU K/AU
L28           6 SEA ABB=ON  PLU=ON  "SRINIVASU K"/AU
                E PATEL N/AU
L29         411 SEA ABB=ON  PLU=ON  ("PATEL N"/AU OR "PATEL N K"/AU OR "PATEL
                N S"/AU)
                E PATEL NILESH/AU
L30           6 SEA ABB=ON  PLU=ON  ("PATEL NILESHKUMAR"/AU OR "PATEL NILESHKUM
                AR SURESHBAI"/AU OR "PATEL NILESHKUMAR SURESHBHAI"/AU OR
                "PATEL NILI"/AU)
                E REJENDRAN C/AU
                D BIB L3
                E CHINAPILLAI R/AU
                E CHINNAPILLAI R/AU
L31           1 SEA ABB=ON  PLU=ON  "CHINNAPILLAI RAJENDRAN"/AU
L32          63 SEA ABB=ON  PLU=ON  (SUN AND PHARM? AND IND?)/CS,PA
L33           2 SEA ABB=ON  PLU=ON  L25 AND (L27 OR L28 OR L29 OR L30 OR L31
                OR L32)
L34          24 SEA ABB=ON  PLU=ON  L25 NOT L32
L35         133 SEA ABB=ON  PLU=ON  L17 OR L19 OR (ISOBENZOFURANCARBONITRILE
                OR ISO (1A) (BENZOFURANCARBONITRILE OR BENZO (1A)(FURANCARBONIT
                RILE OR FURAN (1A) CARBONITRILE)) OR (ISOBENZOFURAN OR
                ISOBENZO (1A) FURAN) (1A) (CARBONITRILE OR CARBO (1A) NITRILE))
                 (2A) FLUOROPHENYL (2A) DIHYDRO
L36           3 SEA ABB=ON  PLU=ON  L35 (2A) (METHYLAMINOPROPYL OR (METHYLAMINO
                 OR METHYL (1A) AMINO) (1A)PROPYL) OR DEMETHYLCITALPRAM# OR
                DEMETHYLCTALOPRAM# OR NORCITALPRAM# OR LU11109 OR LU (1A)
                (11109 OR 11 (1A) 109)
                D SCA
L37           3 SEA ABB=ON  PLU=ON  L34 AND (L35 OR L36)
L38          21 SEA ABB=ON  PLU=ON  (L9 OR ?CITALOPRAM/BI OR CIPRALEX OR
                LEXAPRO OR LU (1A) (260540 OR 26 (1A) 0540 OR 26(1A) 054?) OR
                LU26054? OR LU26 (1A) 540 OR BONITRILE OR LU10171 OR LU10 (1A)
                171 OR LU (1A) (10171 OR 10 (1A) 171) OR NITRALAPRAM OR
                APERTIA OR CELEXA OR CIPRAM) (L) PUR/RL
L39           1 SEA ABB=ON  PLU=ON  L38 AND (L27 OR L28 OR L29 OR L30 OR L31
                OR L32)
L40          20 SEA ABB=ON  PLU=ON  L38 NOT L39
                E CRYSTALLIZ/CT
                E E5+ALL
L41      117878 SEA ABB=ON  PLU=ON  CRYSTALLIZATION+NT/CT
                E E30
                E E3+ALL
L42       89849 SEA ABB=ON  PLU=ON  CRYSTALS+NT/CT
                E PRECIPITATION (CHEMICAL)/CT
                E E3+ALL
L43       25533 SEA ABB=ON  PLU=ON  "PRECIPITATION (CHEMICAL)"+OLD,NT/CT
L44           3 SEA ABB=ON  PLU=ON  L40 AND (L41 OR L42 OR L43)

     FILE 'REGISTRY' ENTERED AT 15:19:08 ON 11 APR 2005.
                E POTASSIUM IODIDE/CN
L45           1 SEA ABB=ON  PLU=ON  "POTASSIUM IODIDE"/CN
                 E CUPROUS CYANIDE/CN
L46           1 SEA ABB=ON  PLU=ON  "CUPROUS CYANIDE"/CN
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                D SCA
L47           18 SEA ABB=ON  PLU=ON  CCUN AND COPPER (1A) CYANIDE
L48           12 SEA ABB=ON  PLU=ON  L47 NOT L6

     FILE 'HCAPLUS' ENTERED AT 15:24:06 ON 11 APR 2005
L49        91001 SEA ABB=ON  PLU=ON  L46 OR ?POTASSIUM/BI (1A) ?IODIDE/BI OR
                 ANTISTRUMIN# OR ASMOFUG# OR CEOIODIN# OR IODOSTIN# OR JODID OR
                 KI OR K1N OR K1 (1A) N OR KAIOD# OR KNOLLIDE OR NSC77632 OR
                 NSC (1A) (77632 OR 77(1A)632) OR PHERAJOD# OR THRYOBLOCK OR
                 THYRO (1A) BLOCK OR THYROJOD#
L50         4727 SEA ABB=ON  PLU=ON  L48 OR (COPPER OR CUPROUS OR CUPRATE) (2A)
                 ?CYANIDE/BI OR CUPRICIN#
L51           24 SEA ABB=ON  PLU=ON  L25 NOT L33
L52            3 SEA ABB=ON  PLU=ON  L51 AND (L35 OR L36)
L53            3 SEA ABB=ON  PLU=ON  L37 OR L52
L54           11 SEA ABB=ON  PLU=ON  L51 AND L49
L55           11 SEA ABB=ON  PLU=ON  L54 AND L50
                 E ALCOHOLS/CT
                 E E3+OLD,NT1
L56              QUE ABB=ON  PLU=ON  ALCOHOLS+OLD,NT1/CT OR ALCOHOL#/CW
                 E ISOPROPANOL/CT
                 E CYCLOHEXANE/CT
                 E E3+ALL
L57        35276 SEA ABB=ON  PLU=ON  CYCLOHEXANE/CT
L58            0 SEA ABB=ON  PLU=ON  L55 AND L56
L59            1 SEA ABB=ON  PLU=ON  L55 AND L57
                 D SCA
                 D COS

     FILE 'REGISTRY' ENTERED AT 15:36:14 ON 11 APR 2005
                 E ISOPROPANOL/CN
L60            1 SEA ABB=ON  PLU=ON  ISOPROPANOL/CN
                 D SCA
L61           71 SEA ABB=ON  PLU=ON  C3H8O AND (ISOPROPANOL OR N-PROPANOL)
L62           26 SEA ABB=ON  PLU=ON  L61 NOT L6
L63           10 SEA ABB=ON  PLU=ON  L62 NOT (MXS/CI OR MIXT)

     FILE 'HCAPLUS' ENTERED AT 15:39:22 ON 11 APR 2005
L64              QUE ABB=ON  PLU=ON  L63 OR ?PROPYL/BI (1A) ALCOHOL OR ?ISOPROP?
                 /BI OR ?PROPANOL/BI OR TIPT OR HYDROXYPROPANE OR ETHYLCARBINOL
                 OR NSC30300 OR NSC (1A) (30300 OR 30 (1A) 300) OR ETHYL (1A)
                 CARBINOL OR OPTAL# OR OSMOSAL OR PROPANOL OR METYLETH? OR
                 ALCOJEL OR ALCOSOLVE
L65         7371 SEA ABB=ON  PLU=ON  AUTOSEPT OR AVANTIN# OR COMBI (1A)SCHUTZ
                 OR COMBISCHUTZ OR DIMETHYLCARBINOL OR (DIMETHYL OR DI (1A)
                 METHYL) (1A) CARBINOL OR HARTOSOL# OR IPA OR IPS OR LUSOL# OR
                 PROPAN (1A) OL OR PETROHOL#
L66           72 SEA ABB=ON  PLU=ON  NSC135801 OR NSC (1A)(135801 OR 135 (1A)
                 801) OR PROPOL# OR STERISOL# OR TAKINEOCOL# OR TOKUSO OR
                 VIRAHOL#
L67            1 SEA ABB=ON  PLU=ON  L55 AND (L64 OR L65 OR L66)
L68            2 SEA ABB=ON  PLU=ON  L59 OR L67
                 D SCA
L69            8 SEA ABB=ON  PLU=ON  L44 OR L53 OR L68
L70            2 SEA ABB=ON  PLU=ON  L33 OR L39

=> b hcap
FILE 'HCAPLUS' ENTERED AT 15:49:06 ON 11 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 11 Apr 2005 VOL 142 ISS 16
FILE LAST UPDATED: 10 Apr 2005 (20050410/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all l70 tot

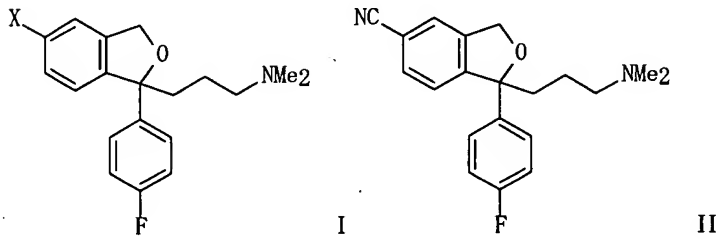
L70 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:1079731 HCAPLUS
DN 142:56160
ED Entered STN: 17 Dec 2004
TI process for purification of citalopram by hydrogenolysis halogenated isobenzofuran impurities
IN Borase, Ashok Punju; **Patel, Nileshkumar Sureshbai**; Kilaru, Srinivasu; Thennati, Rajamannar
PA **Sun Pharmaceuticals Industries** Ltd., **India**
SO Eur. Pat. Appl., 17 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM C07D307-87
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1486492	A2	20041215	EP 2004-291424	20040608
	EP 1486492	A3	20050223		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
	US 2005004380	A1	20050106	US 2004-865139	20040608
PRAI	IN 2003-MU602	A	20030610		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 1486492	ICM	C07D307-87

OS MARPAT 142:56160
GI



AB The present invention provides a process for decreasing the content of halogenated isobenzofuran impurities I (X = halo) in citalopram (II) by hydrogenolysis to I (X = H). Thus, 5 g crude citalopram base containing 4.84% of bromo impurity I (X = Br) is dissolved in 50 mL EtOAc, 0.1 g Pd/C and 0.1 g sodium hypophosphite added and the mixture refluxed for 2 h. Anal. showed that the bromo impurity I (X = Br) is absent.
ST citalopram purifn hydrogenolysis halogenated isobenzofuran impurity
IT Hydrogenolysis
(process for purification of citalopram by hydrogenolysis halogenated impurities)
IT Alcohols, uses

RL: NUU (Other use, unclassified); USES (Uses)
(solvent; process for purification of citalopram by hydrogenolysis halogenated impurities)

IT 7440-02-0, Nickel, uses 7440-05-3, Palladium, uses 7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses
RL: CAT (Catalyst use); USES (Uses)
(process for purification of citalopram by hydrogenolysis halogenated impurities)

IT **59729-32-7P, Citalopram** hydrobromide **59729-33-8P, Citalopram 207559-01-1P, Citalopram** oxalate
RL: **PUR (Purification or recovery); PREP (Preparation)**
(process for purification of **citalopram** by hydrogenolysis halogenated impurities)

IT **64169-39-7**
RL: RCT (Reactant); REM (Removal or disposal); PROC (Process); RACT (Reactant or reagent)
(process for purification of citalopram by hydrogenolysis halogenated impurities)

IT 540-69-2, Ammonium formate 1333-74-0, Hydrogen, reactions 7681-53-0, Sodium hypophosphite
RL: RGT (Reagent); RACT (Reactant or reagent)
(process for purification of citalopram by hydrogenolysis halogenated impurities)

IT 390817-87-5P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(process for purification of **citalopram** by hydrogenolysis halogenated impurities)

IT 75-09-2, Dichloromethane, uses 141-78-6, Ethyl acetate, uses 7732-18-5, Water, uses
RL: NUU (Other use, unclassified); USES (Uses)
(solvent; process for purification of citalopram by hydrogenolysis halogenated impurities)

L70 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:551309 HCAPLUS
DN 139:117333
ED Entered STN: 18 Jul 2003
TI Process for the preparation of 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile via cyanation of the corresponding chloride or bromide precursors.
IN Thennati, Rajamannar; Kilaru, Srinivasu; **Chinnapillai, Rajendran**; **Patel, Nileshkumar Sureshbhai**
PA **Sun Pharmaceutical Industries** Limited, **India**
SO PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003057132	A2	20030717	WO 2003-IN6	20030107
	WO 2003057132	A3	20040226		
	WO 2003057132	C1	20040415		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2005043550	A1	20050224	US 2004-500532	20040719
PRAI	IN 2002-MU10	A	20020107		
	IN 2002-MU18	A	20020110		

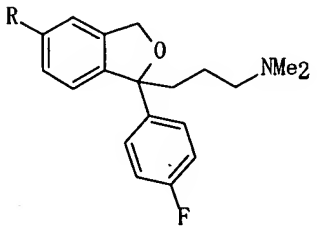
IN 2002-MU847 A 20020930
WO 2003-IN6 W 20030107

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2003057132	ICM	A61K
US 2005043550	ECLA	C07D307/87B

OS CASREACT 139:117333; MARPAT 139:117333

GI



I

AB Title compound (I; R = cyano) (citalopram) was prepared by treatment of I (R = Cl, Br) with a cyanide source in the presence of I- in an amide, amine, or polyether solvent followed by treatment of the crude product containing 1-[3-(methylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile and 5-carboxamido-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)phthalide impurities with a phosphorus oxyhalide, phosphorus oxide cyanide reversal agent, and purification using a solvent system comprising a hydrocarbon and alc., ester, ether, ketone, or mixture thereof. Thus, citalopram containing 4.7% amide and 0.72% desmethylcitalopram impurities was heated with POCl3 in PhMe at 70° for 1 h. The mixture was poured into water and pH was adjusted to 2.0-2.5 with aqueous HCl. The PhMe layer was separated and the pH of the aqueous layer was adjusted to 9.0-9.5 with aqueous NH3 followed by extraction with PhMe to give product containing 0.05% and 0.23% of the amide and desmethylcitalopram resp.

ST citalopram prepn purifn phosphorus oxychloride; halodimethylaminopropylfluorophenyldihydroisobenzofuran cyanation

IT Solvents
(halogenated; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

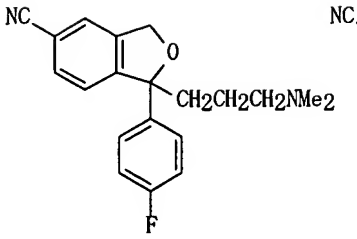
IT Cyanation catalysts
(iodide ion; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

IT Iodides, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(metal iodides; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

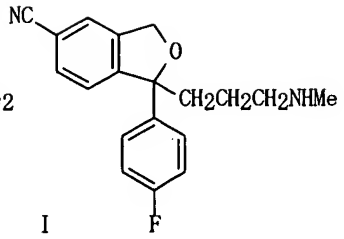
IT Cyanation
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

IT Alcohols, uses
Amides, uses
Amines, uses
Aromatic hydrocarbons, uses
Esters, uses
Ethers, uses
Hydrocarbons, uses
Ketones, uses
Nitriles, uses
Nitro compounds
Polyethers, uses
RL: NUU (Other use, unclassified); USES (Uses)
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

IT 62498-67-3P 64372-56-1P
RL: **BYP (Byproduct); PREP (Preparation)**
(process for the preparation of **citalopram** via cyanation of the corresponding chloride or bromide precursor)



I



II

AB The present invention relates to an industrially advantageous method for the purification of citalopram (I) wherein desmethyl citalopram (II), present in crude citalopram as an impurity, is methylated to produce pure citalopram I. The resulting citalopram product I is isolated as the base or a pharmaceutically acceptable salt thereof. Thus, to crude citalopram (90 g, 0.28 mol) containing desmethyl citalopram (7 %, HPLC), formic acid (98%, 2.7 g) was added followed by aqueous formaldehyde(35%, 2.37 g). The reaction mass was heated at 85-95° for 30 min, cooled to 30° , and diluted with ethanol (900 mL), treated with oxalic acid dihydrate (41.94 g, 0.33 mol), and heated to reflux. The obtained solution was cooled to 20-25° and stirring was continued for 2 h at 20-25° , followed by collecting the product by filtration and recrystn. from ethanol to give highly pure 92 g crystalline citalopram oxalate having HPLC purity 99.7% wherein desmethyl citalopram (impurity) was not detected.

ST methylation desmethyl citalopram formaldehyde formic acid; citalopram prepn

IT **62498-67-3P**, Desmethyl **citalopram**
RL: **BYP (Byproduct)**; RCT (Reactant); **PREP (Preparation)**
; RACT (Reactant or reagent)
(preparation of pure **citalopram** by N-methylation of crude **citalopram** containing desmethyl **citalopram** with formaldehyde and formic acid)

IT **59729-33-8P, Citalopram**
RL: **IMF (Industrial manufacture)**; **PUR (Purification or recovery)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of pure **citalopram** by N-methylation of crude **citalopram** containing desmethyl **citalopram** with formaldehyde and formic acid)

IT **59729-32-7P, Citalopram** Hydrobromide
RL: **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of pure **citalopram** by N-methylation of crude **citalopram** containing desmethyl **citalopram** with formaldehyde and formic acid)

IT 64-18-6, Formic acid, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of pure citalopram by N-methylation of crude citalopram containing desmethyl citalopram with formaldehyde and formic acid)

IT 50-00-0, Formaldehyde, reactions 544-92-3, Cuprous cyanide 6153-56-6, Oxalic acid dihydrate 10035-10-6, Hydrobromic acid, reactions **64169-39-7**, 5-Bromo-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran 207559-01-1, Citalopram oxalate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of pure citalopram by N-methylation of crude citalopram containing desmethyl citalopram with formaldehyde and formic acid)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Petersen; US 6258842 B1 2001 HCAPLUS
(2) Petersen; US 6291689 B1 2001 HCAPLUS

IT **62498-67-3P**, Desmethyl **citalopram**
RL: **BYP (Byproduct)**; RCT (Reactant); **PREP (Preparation)**
; RACT (Reactant or reagent)
(preparation of pure **citalopram** by N-methylation of crude

citalopram containing desmethyl **citalopram** with formaldehyde and formic acid)

IT **59729-33-8P, Citalopram**
RL: **IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)**
(preparation of pure **citalopram** by N-methylation of crude **citalopram** containing desmethyl **citalopram** with formaldehyde and formic acid)

IT **59729-32-7P, Citalopram** Hydrobromide
RL: **IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)**
(preparation of pure **citalopram** by N-methylation of crude **citalopram** containing desmethyl **citalopram** with formaldehyde and formic acid)

IT **64169-39-7**, 5-Bromo-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of pure citalopram by N-methylation of crude citalopram containing desmethyl citalopram with formaldehyde and formic acid)

L69 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:546472 HCAPLUS
DN 141:106278
ED Entered STN: 08 Jul 2004
TI A process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram
IN Petersen, Hans; Dancer, Robert; Christiansen, Brian; Humble, Rikke Eva
PA H. Lundbeck A/S, Den.
SO PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07C253-34
ICS C07D307-87
CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 45, 48
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004056754	A1	20040708	WO 2003-DK907	20031218

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI DK 2002-2004	A	20021223	
US 2002-436117P	P	20021223	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004056754	ICM	C07C253-34
	ICS	C07D307-87

AB The invention relates to a process for the preparation of racemic citalopram diol [i.e., citalopram diol means 4-[4-(dimethylamino)-1-(4-fluorophenyl)-1-hydroxybutyl]-3-(hydroxymethyl)benzonitrile] and/or R- or S-citalopram diol, comprising the separation of a non-racemic mixture of R- and S-citalopram diol with more than 50% of one of the enantiomers into a fraction being enriched with S- or R-citalopram diol and a fraction comprising RS-citalopram diol wherein the ratio of R-citalopram diol:S-citalopram diol is equal to 1:1 or closer to 1:1 than in the initial mixture The method is characterized in that (i) RS-citalopram diol is precipitated from a solution of the initial non-racemic mixture, or R- or S-citalopram diol is

dissolved into a solvent from the initial non-racemic mixture, leaving a residue of RS-citalopram diol, and in that (ii) the residue/precipitate formed is separated from the final solution phase, followed by optional steps of repetition, recrystn., purification, isolation and conversion between free base and salts. The invention also relates to a process for the preparation of RS-citalopram, S-citalopram or R-citalopram (all as free base and/or acid addition salt) comprising the method described above followed by ring closure.

ST citalopram diol racemic prepn

IT **Crystallization**
Neutralization
Precipitation (chemical)
Recrystallization
Resolution (separation)
(process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)

IT Alcohols, uses
Ketones, uses
RL: NUU (Other use, unclassified); USES (Uses)
(solvents; process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)

IT 481047-48-7P 488787-59-3P
RL: **PUR (Purification or recovery)**; PREP (Preparation)
(process for the preparation of racemic **citalopram** diol and/or S- or R-**citalopram** diols and the use of such diols for the preparation of racemic **citalopram** R-**citalopram** and/or S-**citalopram**)

IT 64-19-7, Acetic acid, reactions 75-75-2, Methanesulfonic acid 104-15-4, reactions 144-62-7, Oxalic acid, reactions 7647-01-0, Hydrogen chloride, reactions 7664-93-9, Sulfuric acid, reactions 10035-10-6, Hydrogen bromide, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)

IT 103146-25-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)

IT 717133-25-0P 717133-26-1P 717133-27-2P 717133-28-3P 717133-29-4P 717133-30-7P 717133-31-8P 717133-32-9P 717909-60-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)

IT 60-29-7, Ethyl ether, uses 67-63-0, 2-Propanol, uses 67-64-1, Acetone, uses 75-05-8, Acetonitrile, uses 108-10-1, Methyl isobutyl ketone 108-88-3, Toluene, uses 109-99-9, Thf, uses 141-78-6, Ethyl acetate, uses 7732-18-5, Water, uses
RL: NUU (Other use, unclassified); USES (Uses)
(solvent; process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) H Lundbeck AS; EP 0347066 A1 1989 HCAPLUS
(2) H Lundbeck AS; WO 03000672 A1 2003 HCAPLUS

L69 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:777773 HCAPLUS
DN 139:276808
ED Entered STN: 03 Oct 2003
TI Transalification process for the preparation of purified citalopram hydrochloride or hydrobromide
IN Hamied, Yusuf Khwaja; Kankan, Rajendra N.; Rao, Dharmaraj R.
PA Cipla Ltd., India; Wain, Christopher Paul

SO PCT Int. Appl., 10 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D307-87
ICS A61K031-343
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 45, 48, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003080589	A1	20031002	WO 2003-GB1032	20030311
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1485367	A1	20041215	EP 2003-708344	20030311
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003008603	A	20050209	BR 2003-8603	20030311
PRAI GB 2002-6708	A	20020321		
WO 2003-GB1032	W	20030311		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2003080589	ICM	C07D307-87
	ICS	A61K031-343

AB Purified citalopram hydrochloride or hydrobromide are made by purifying another different citalopram salt (e.g., citalopram besylate by crystallization) and then converting the purified salt to the hydrochloride or hydrobromide.

ST transalification prepn citalopram hydrochloride; hydrobromide citalopram transalification prepn; crystn transalification prepn citalopram hydrobromide

IT **Crystallization**
(in a transalification process for the preparation of purified citalopram hydrochloride or hydrobromide)

IT 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-64-1, Acetone, uses 78-93-3, MEK, uses 108-10-1, MIBK 108-88-3, Toluene, uses 110-54-3, Hexane, uses 141-78-6, Ethyl acetate, uses 142-82-5, Heptane, uses 7732-18-5, Water, uses
RL: NUU (Other use, unclassified); USES (Uses)
(crystallization solvent; in a transalification process for the preparation of purified citalopram hydrochloride or hydrobromide)

IT 606932-12-1P
RL: **PUR (Purification or recovery)**; RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(transalification process for the preparation of purified **citalopram** hydrochloride or hydrobromide)

IT 98-11-3, Benzenesulfonic acid, reactions 59729-33-8, Citalopram
RL: RCT (Reactant); RACT (Reactant or reagent)
(transalification process for the preparation of purified citalopram hydrochloride or hydrobromide)

IT 59729-32-7P, Citalopram hydrobromide 85118-27-0P, Citalopram hydrochloride
RL: SPN (Synthetic preparation); PREP (Preparation)
(transalification process for the preparation of purified citalopram hydrochloride or hydrobromide)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Liljegren, K; WO 0180619 A 2001 HCAPLUS
(2) Paul, W; WO 02070501 A 2002 HCAPLUS
(3) Petersen, H; WO 0168627 A 2001
(4) Sumika Fine Chemicals Co Ltd; EP 1152000 A 2001 HCAPLUS

L69 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:590880 HCAPLUS
DN 139:133459
ED Entered STN: 01 Aug 2003
TI Cyanation process for the preparation of citalopram and its extractive purification
IN Coppi, Laura; Gasanz Guillen, Yolanda; Campon Pardo, Julio
PA Esteve Quimica, S.A., Spain
SO U.S. Pat. Appl. Publ., 5 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM C07D307-87
NCL 549467000
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 45, 48
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003144534	A1	20030731	US 2003-351289	20030124
	US 6635773	B2	20031021		
	ES 2194597	A1	20031116	ES 2002-167	20020125
	ES 2194597	B2	20040801		
	WO 2003062218	A1	20030731	WO 2003-ES37	20030124
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1479673	A1	20041124	EP 2003-706634	20030124
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRAI	ES 2002-167	A	20020125		
	WO 2003-ES37	W	20030124		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2003144534	ICM	C07D307-87
	NCL	549467000
US 2003144534	ECLA	C07D307/87B
EP 1479673	ECLA	C07D307/87B

AB Crude citalopram was prepared the cyanation of 1-[3-(dimethylamine)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-bromoisobenzofuran with **copper cyanide** and purified citalopram or one of its salts (e.g., citalopram hydrobromide) was obtained by the extractive purification of citalopram by selective extns. of citalopram or it salts of its impurities with organic solvents (e.g., toluene and heptane) and water under specific conditions of pH and temperature
ST citalopram prepn extractive purifn; hydrobromide citalopram prepn extractive purifn
IT Extraction
(cyanation process for the preparation of citalopram and its extractive purification)
IT Cyanation
(cyanation process using **copper cyanide** and 1-[3-(dimethylamine)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-bromoisobenzofuran for the preparation of citalopram and its extractive purification)
IT Aromatic hydrocarbons, uses
RL: NUU (Other use, unclassified); USES (Uses)
(extraction solvents; in a cyanation process for the preparation of citalopram and its extractive purification)
IT Neutralization
(of citalopram base with acids in the preparation of citalopram salts)

IT **59729-33-8P, Citalopram**
RL: **PUR (Purification or recovery)**; RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(cyanation process for the preparation of **citalopram** and its extractive purification)
IT **544-92-3, Copper cyanide 64169-39-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation process for the preparation of citalopram and its extractive purification)
IT **59729-32-7P, Citalopram** hydrobromide
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(cyanation process for the preparation of **citalopram** and its extractive purification)
IT 108-88-3, Toluene, uses 110-54-3, Hexane, uses **110-82-7**, Cyclohexane, uses 142-82-5, Heptane, uses 1330-20-7, Xylene, uses
RL: NUU (Other use, unclassified); USES (Uses)
(extraction solvent; in a cyanation process for the preparation of citalopram and its extractive purification)
IT 10035-10-6, Hydrogen bromide, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(in the preparation of citalopram hydrobromide)
IT 7732-18-5, Water, uses
RL: NUU (Other use, unclassified); USES (Uses)
(solvent; cyanation process for the preparation of citalopram and its extractive purification)
IT **59729-33-8P, Citalopram**
RL: **PUR (Purification or recovery)**; RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(cyanation process for the preparation of **citalopram** and its extractive purification)
IT **544-92-3, Copper cyanide 64169-39-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation process for the preparation of citalopram and its extractive purification)
IT **59729-32-7P, Citalopram** hydrobromide
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(cyanation process for the preparation of **citalopram** and its extractive purification)
IT **110-82-7**, Cyclohexane, uses
RL: NUU (Other use, unclassified); USES (Uses)
(extraction solvent; in a cyanation process for the preparation of citalopram and its extractive purification)

L69 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:32670 HCAPLUS
DN 138:55856
ED Entered STN: 15 Jan 2003
TI Process for the preparation of highly pure salts of citalopram
IN Satyanarayana, Chava; Venkata, Ramana Rao Chunchu; Jyothi, Basu Abbineni; Hari, Babu Bobepudi
PA Matrix Laboratories Limited, India
SO Brit. UK Pat. Appl., 18 pp.
CODEN: BAXXDU
DT Patent
LA English
IC ICM C07D307-87
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 2375763	A1	20021127	GB 2002-10225	20020503
	GB 2375763	B2	20030924		
	CA 2444940	AA	20030904	CA 2002-2444940	20020418
	WO 2003072565	A1	20030904	WO 2002-IB3832	20020418
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				

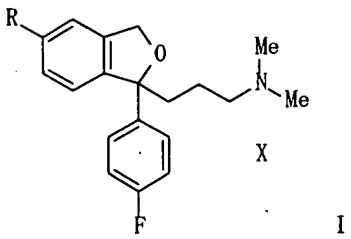
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,
GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,
GN, GQ, GW, ML, MR, NE, SN, TD, TG

BR	2002009194	A	20040608	BR 2002-9194	20020418
EP	1478635	A1	20041124	EP 2002-806883	20020418
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
GB	2387596	A1	20031022	GB 2003-15853	20020503
GB	2387596	B2	20040211		
GB	2387844	A1	20031029	GB 2003-15852	20020503
ZA	2003008115	A	20040705	ZA 2003-8115	20031017
PRAI GB	2002-4607	A	20020227		
WO	2002-IB3832	W	20020418		
GB	2002-10225	A	20020503		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
GB 2375763	ICM	C07D307-87
GB 2375763	ECLA	C07D209/44; C07D307/87B
GB 2387596	ECLA	C07D307/87B
GB 2387844	ECLA	C07D209/44; C07D307/87B

GI



I

AB A process for preparing highly pure salts of citalopram, such as I (R = CN; X = oxalate, hydrobromide, hydrochloride), for pharmaceutical compns. was described. Thus, citalopram contaminated with up to 5.0% of desmethyl citalopram was added to acetone and stirred for 15 min at 40° followed by addn of oxalic acid to form citalopram oxalate in 85% yield with desmethyl citalopram content <0.1%.

ST citalopram salt prepn

IT **59729-33-8P, Citalopram 207559-01-1P, Citalopram** oxalate
RL: **IMF (Industrial manufacture)**; **PUR (Purification or recovery)**; RCT (Reactant); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(process for the preparation of highly pure salts of **citalopram**)

IT **85118-27-0P, Citalopram** hydrochloride
RL: **IMF (Industrial manufacture)**; **PUR (Purification or recovery)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(process for the preparation of highly pure salts of **citalopram**)

IT **59729-32-7P, Citalopram** hydrobromide
RL: **IMF (Industrial manufacture)**; **PUR (Purification or recovery)**; **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(process for the preparation of highly pure salts of **citalopram**)

IT 67-64-1, Acetone, uses 108-20-3, Isopropyl ether 108-88-3, Toluene, uses 110-54-3, Hexane, uses 110-82-7, Cyclohexane, uses 142-82-5, Heptane, uses 1330-20-7, Xylene, uses

RL: NUU (Other use, unclassified); USES (Uses)
(process for the preparation of highly pure salts of citalopram)

IT 144-62-7, Oxalic acid, reactions 7647-01-0, Hydrochloric acid, reactions 7664-41-7, Ammonia, reactions 10035-10-6, Hydrobromic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the preparation of highly pure salts of citalopram)

IT **62498-67-3**, Desmethyl citalopram **64169-39-7** **64169-45-5** **64372-56-1**
RL: REM (Removal or disposal); PROC (Process)
(process for the preparation of highly pure salts of citalopram)

IT **59729-33-8P**, **Citalopram** **207559-01-1P**, **Citalopram** oxalate
RL: **IMF (Industrial manufacture)**; **PUR (Purification or recovery)**; RCT (Reactant); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(process for the preparation of highly pure salts of **citalopram**)

IT **85118-27-0P**, **Citalopram** hydrochloride
RL: **IMF (Industrial manufacture)**; **PUR (Purification or recovery)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(process for the preparation of highly pure salts of **citalopram**)

IT **59729-32-7P**, **Citalopram** hydrobromide
RL: **IMF (Industrial manufacture)**; **PUR (Purification or recovery)**; **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(process for the preparation of highly pure salts of **citalopram**)

IT **62498-67-3**, Desmethyl citalopram **64169-39-7** **64169-45-5** **64372-56-1**
RL: REM (Removal or disposal); PROC (Process)
(process for the preparation of highly pure salts of citalopram)

L69 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:716262 HCAPLUS
DN 137:232543
ED Entered STN: 20 Sep 2002
TI Cyanation process for the preparation of citalopram
IN Biswas, Sujay; Sharma, Tarun Kant; Kumar, Yatendra; Sathyanarayana, Swargam; Vijayaraghavan, Bakthavathsalan
PA Ranbaxy Laboratories Limited, India
SO PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D307-77
ICS C07D307-81
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 45
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002072565	A1	20020919	WO 2002-IB690	20020308
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2439856	AA	20020919	CA 2002-2439856	20020308
	EP 1370545	A1	20031217	EP 2002-702634	20020308
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	BR 2002007895	A	20041228	BR 2002-7895	20020308
	JP 2005500256	T2	20050106	JP 2002-571481	20020308
PRAI	IN 2001-DE264	A	20010309		
	WO 2002-IB690	W	20020308		

CLASS
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

WO 2002072565 ICM C07D307-77
ICS C07D307-81

OS CASREACT 137:232543

AB An improved and industrially advantageous process for the preparation of citalopram and pharmaceutically acceptable acid addition salts consists of reacting a precursor substituted with a bromo or an iodo group in the same position as the cyano group in citalopram with a cyanide source in a solvent in the present of a N-containing base; the citalopram free base may then be salified with a pharmaceutically acceptable acids.

ST citalopram prepn cyanation process

IT Amines, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(bases; in the formation of complexes with cyanide sources for the cyanation of 1-(4'-fluorophenyl)-1-(3-dimethylaminopropyl)-5-iodo-or-bromophthalane into citalopram)

IT Antidepressants
(cyanation process for the preparation of citalopram)

IT Mental disorder
(depression; cyanation process for the preparation of citalopram for the treatment of)

IT Cyanation
(of 1-(4'-fluorophenyl)-1-(3-dimethylaminopropyl)-5-iodo-or-bromophthalane with a complex of a cyanide source with a base)

IT Neutralization
(of citalopram base with pharmaceutically acceptable acids)

IT 62-53-3, Aniline, reactions 75-50-3, Trimethylamine, reactions 91-22-5, Quinoline, reactions 101-83-7, Dicyclohexylamine 108-18-9, **Diisopropylamine** 108-48-5, 2,6-Lutidine 108-89-4, 4-Methylpyridine 110-86-1, Pyridine, reactions 121-44-8, Triethylamine, reactions 6674-22-2, DBU
RL: RGT (Reagent); RACT (Reactant or reagent)
(base; in the formation of complexes with cyanide sources for the cyanation of 1-(4'-fluorophenyl)-1-(3-dimethylaminopropyl)-5-iodo-or-bromophthalane into citalopram)

IT **59729-32-7P, Citalopram** hydrobromide **59729-33-8P, Citalopram**
RL: **IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)**
(cyanation process for the preparation of **citalopram**)

IT 7732-18-5, Water, uses 10035-10-6, Hydrogen bromide, uses
RL: NUU (Other use, unclassified); REM (Removal or disposal); PROC (Process); USES (Uses)
(cyanation process for the preparation of citalopram HBr from)

IT **64169-39-7** 260066-78-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation process for the preparation of citalopram from)

IT 143-33-9, Sodium cyanide 151-50-8, Potassium cyanide **544-92-3, Cuprous cyanide** 557-21-1, Zinc cyanide 12211-52-8, Ammonium cyanide
RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent)
(cyanation process for the preparation of citalopram from)

IT 68-12-2, Dmf, uses 127-19-5, Dimethylacetamide 872-50-4, N-Methylpyrrolidone, uses 931-20-4, N-Methylpiperidone 1690-76-2
RL: NUU (Other use, unclassified); REM (Removal or disposal); PROC (Process); USES (Uses)
(solvent; cyanation process for the preparation of citalopram)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Bogeso; US 4136193 A 1979 HCAPLUS
(2) Lundbeck, H; WO 0011926 A2 2000
(3) Lundbeck, H; WO 0013648 A2 2000 HCAPLUS

IT **59729-32-7P, Citalopram** hydrobromide **59729-33-8P, Citalopram**
RL: **IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)**
(cyanation process for the preparation of **citalopram**)

IT **64169-39-7**

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation process for the preparation of citalopram from)

IT **544-92-3, Cuprous cyanide**
RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent)
(cyanation process for the preparation of citalopram from)

L69 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:472398 HCAPLUS
DN 135:61224
ED Entered STN: 29 Jun 2001
TI Method for the preparation and purification of citalopram
IN Villa, Marcos; Sbrogio, Federico; Dancer, Robert
PA H. Lundbeck A/S, Den.
SO PCT Int. Appl., 12 pp.
CODEN: PIXXD2
DT Patent
LA English
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 45
FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001045483	A2	20010628	WO 2001-DK147	20010307
	WO 2001045483	A3	20011227		
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	NL 1017525	C1	20010426	NL 2001-1017525	20010307
	CA 2360303	AA	20010628	CA 2001-2360303	20010307
	CA 2360303	C	20030812		
	EP 1181713	A2	20020227	EP 2001-913726	20010307
	EP 1181713	B1	20040929		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	TR 200201166	T1	20021021	TR 2002-200201166	20010307
	JP 2003517484	T2	20030527	JP 2001-546230	20010307
	BR 2001006272	A	20040615	BR 2001-6272	20010307
	EP 1462447	A2	20040929	EP 2004-4482	20010307
	EP 1462447	A3	20041117		
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	AT 277920	E	20041015	AT 2001-913726	20010307
	DK 174018	B1	20020422	DK 2001-402	20010308
	GB 2357763	A1	20010704	GB 2001-5983	20010312
	GB 2357763	B2	20020116		
	GB 2359811	A1	20010905	GB 2001-15025	20010312
	GB 2359811	B2	20030305		
	CZ 292200	B6	20030813	CZ 2001-890	20010312
	FI 108639	B1	20020228	FI 2001-500	20010313
	NO 312462	B1	20020513	NO 2001-1271	20010313
	FR 2812877	A1	20020215	FR 2001-3455	20010314
	FR 2812877	B1	20030404		
	GR 1003874	B1	20020424	GR 2001-100132	20010316
	DE 10112829	C1	20020725	DE 2001-10112829	20010316
	CH 691535	A	20010815	CH 2001-545	20010322
	BE 1013212	A6	20011002	BE 2001-188	20010322
	NL 1018360	C1	20011004	NL 2001-1018360	20010622
	BE 1013213	A6	20011002	BE 2001-435	20010626
	CH 691998	A	20011231	CH 2001-1411	20010726
	ES 2170732	A1	20020801	ES 2001-1762	20010727
	AU 744112	B1	20020214	AU 2001-65477	20010827
	SE 517623	C2	20020625	SE 2001-3045	20010914
	SE 2001003045	A	20020623		

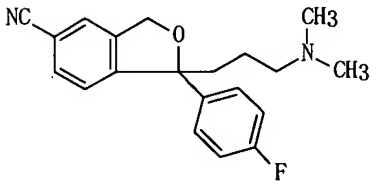
	BG 106203	A	20020830	BG 2001-106203	20011210
	ZA 2001010179	A	20021211	ZA 2001-10179	20011211
	NZ 516298	A	20021220	NZ 2001-516298	20011220
	HR 2002000004	A1	20030430	HR 2002-4	20020104
	US 2002120005	A1	20020829	US 2002-46126	20020108
	US 6455710	B2	20020924		
PRAI	DK 2000-1929	A	20001222		
	NL 2001-1017525	A	20001222		
	EP 2001-913726	A3	20010307		
	WO 2001-DK147	W	20010307		
	GB 2001-5983	A3	20010312		
	CH 2001-545	A	20010322		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2001045483		
NL 1017525	ECLA	C07D307/87B
EP 1462447	ECLA	C07D307/87B
GB 2357763	ECLA	C07D307/87B
GB 2359811	ECLA	C07D307/87B
FR 2812877	ECLA	C07D307/87B
DE 10112829	ECLA	C07D307/87B
CH 691535	ECLA	C07D307/87B
BE 1013212	ECLA	C07D307/87B
NL 1018360	ECLA	C07D307/87B
BE 1013213	ECLA	C07D307/87B
CH 691998	ECLA	C07D307/87B
US 2002120005	ECLA	C07D307/87B

OS CASREACT 135:61224; MARPAT 135:61224

GI



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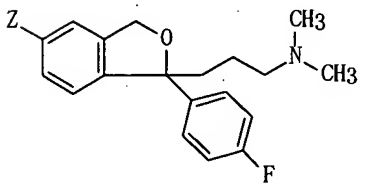


II

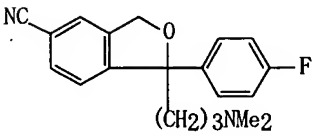
AB A process for the preparation and purification of citalopram (I) is presented in which a benzoisofuran derivative [II; Z = iodo, bromo, chloro, CF3(CF2)nSO2O; n = 0-8] is subjected to a cyanide-exchange reaction with a cyanide source (e.g., cuprous cyanide). The resultant crude citalopram is optionally subjected to some initial purification and subsequently treated with an amide or an amide-like group forming agent (e.g., acetic anhydride), the reaction mixture is then subjected to an acid/base wash and/or crystallization and recrystn. of citalopram in order to remove the amides formed from the crude citalopram mixture, and the resulting citalopram product is optionally further purified, worked up and isolated as the base or a pharmaceutically acceptable salt.

ST citalopram prepn purifn

IT **Crystallization**
Recrystallization
Washing
(method for the preparation and purification of citalopram using)

IT Acids, reactions
Bases, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(method for the preparation and purification of citalopram using a washing with)
IT Carbonitriding
(method for the preparation of citalopram using)
IT Amidation
(method for the purification of citalopram using)
IT Acid halides
Anhydrides
RL: RCT (Reactant); RACT (Reactant or reagent)
(method for the purification of citalopram using amide-forming)
IT 7440-02-0, Nickel, uses 7440-05-3, Palladium, uses 7440-50-8, Copper, uses 7440-66-6, Zinc, uses
RL: CAT (Catalyst use); USES (Uses)
(cyanidation catalyst for the preparation of citalopram)
IT **59729-33-8P, Citalopram**
RL: IMF (Industrial manufacture); **PUR (Purification or recovery)**; SPN (Synthetic preparation); PREP (Preparation)
(method for the preparation and purification of **citalopram**)
IT 64169-39-7 64169-45-5 260066-78-2 260066-82-8 345658-19-7 345658-20-0 345658-21-1 345658-22-2 345658-23-3 345658-24-4 345658-25-5 345658-26-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(method for the preparation of citalopram by the cyanidation of)
IT 544-92-3, Cuprous cyanide 557-21-1, Zinc cyanide
RL: RCT (Reactant); RACT (Reactant or reagent)
(method for the preparation of citalopram using)
IT 75-36-5, Acetyl chloride 108-24-7, Acetic anhydride
RL: RCT (Reactant); RACT (Reactant or reagent)
(method for the purification of crude citalopram by reaction of the crude reaction mixture with)
IT **59729-33-8P, Citalopram**
RL: IMF (Industrial manufacture); **PUR (Purification or recovery)**; SPN (Synthetic preparation); PREP (Preparation)
(method for the preparation and purification of **citalopram**)

L69 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1977:561413 HCAPLUS
DN 87:161413
ED Entered STN: 12 May 1984
TI Quantitative structure-activity relationships in a series of selective 5-HT uptake inhibitors
AU Bigler, Allan J.; Boegesoe, Klaus P.; Toft, Anders; Hansen, Villy
CS Dep. Synth. Chem., H. Lundbeck and Co. A/S, Copenhagen-Valby, Den.
SO European Journal of Medicinal Chemistry (1977), 12(3), 289-95
CODEN: EJMCA5; ISSN: 0223-5234
DT Journal
LA English
CC 1-3 (Pharmacodynamics)
Section cross-reference(s): 27
OS CASREACT 87:161413
GI



HBr I

AB Fifty-five 1-[3-(methylamino)propyl]- and 1-[3-(dimethylamino)propyl]-1-phenylphthalan derivs. were prepared and tested in vitro for inhibition of 5-hydroxytryptamine [50-67-9] uptake in blood platelets and in vivo for potentiation of 5-HTP syndrome in mice. Quant. structure-activity relations were established, using the methods of Free-Wilson and Hansch.

Of several potent compds., Citalopram (I) [59729-33-8] was the most active.

ST hydroxytryptamine inhibitor phthalan deriv

IT Substituent effect
(on (dimethylaminopropyl) phenylphthalan derivs. inhibition of hydroxytryptamine)

IT Molecular structure-biological activity relationship
(hydroxytryptamine-inhibiting, of (dimethylaminopropyl) phenylphthalans)

IT Substituent constant
(π, of (dimethylaminopropyl) phenylphthalan derivs., lipophilicity in relation to)

IT 109-54-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with benzophenone derivative)

IT 74-96-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with phthalancarbonitrile derivative)

IT 460-00-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with phthalide derivative)

IT 789-96-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of)

IT 50-67-9, biological studies
RL: BIOL (Biological study)
(inhibition of, by (dimethylaminopropyl) phenylphthalans)

IT 64372-57-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and Grignard reaction with bromobenzene derivative)

IT 64372-58-3P 64372-61-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and Grignard reaction with propyl chloride derivs.)

IT 64169-67-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkylation of)

IT 64169-66-0P 64372-62-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyanation of)

IT 64169-65-9P 64372-59-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

IT 64372-63-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 10565-62-5P 10588-99-5P **59729-33-8P** **62498-68-4P**
62498-70-8P 64169-43-3P **64169-47-7P** 64169-54-6P
64169-58-0P 64349-04-8P 64371-94-4P 64371-95-5P 64371-97-7P
64371-98-8P 64371-99-9P 64372-01-6P 64372-02-7P 64372-03-8P
64372-04-9P 64372-05-0P 64372-07-2P 64372-09-4P 64372-11-8P
64372-13-0P 64372-14-1P 64372-15-2P 64372-16-3P 64372-18-5P
64372-20-9P 64372-21-0P 64372-23-2P 64372-25-4P 64372-27-6P
64372-28-7P 64372-29-8P 64372-31-2P 64372-32-3P 64372-34-5P
64372-36-7P 64372-37-8P 64372-39-0P 64372-41-4P 64372-42-5P
64372-43-6P 64372-44-7P 64372-45-8P 64372-47-0P
64372-48-1P 64372-49-2P **64372-51-6P** 64372-53-8P
64372-54-9P 64372-55-0P **64372-56-1P** 64406-38-8P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation and hydroxytryptamine inhibition by)

IT 64372-60-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

IT 64169-52-4P 64372-08-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 657-06-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
IT 64169-64-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
IT **59729-33-8P 62498-68-4P 64169-47-7P**
64372-43-6P 64372-51-6P 64372-56-1P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation and hydroxytryptamine inhibition by)

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